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STUDY OF EFFECTS OF INJECTOR GEOMETRY
ON FUEL-AIR MIXING AND COMBUSTION

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Prepared for

NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

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ABSTRACT

An implicit finite-difference method has been developed for computing the flow in the near field of a fuel injector. This work was done as part of a broader study of the effects of fuel injector geometry on fuel-air mixing and combustion. Detailed numerical results have been obtained for cases of laminar and turbulent flow without base injection, corresponding to the supersonic base flow problem. These numerical results indicated that the method is stable and convergent, and that significant savings in computer time can be achieved, compared with explicit methods.

1.0 INTRODUCTION

This research program involved experiments and analysis to relate characteristics of fuel injector geometry to the fuel-air mixing and combustion. The original experimental program has been only partially completed at this time, because of numerous mechanical difficulties in the test facility and the instrumentation. References 1-3 give details of the experimental plan and also describe most of the experimental results and conclusions obtained to this point. In developing computational methods for the turbulent mixing and reacting flow, it became necessary to model the time-average rate of fuel consumption by chemical reaction at each point in the flow. References 3 and 4 describe the main results of this effort.

The present report is concerned with the last phase of the research program, which was the development of a numerical method for computing the flow properties in the near field of a fuel injector. This effort was a natural part of a study of effects of injector geometry on fuel-air mixing and combustion, because the principal effects of changes in injector geometry occur in the near field of the injector. This near field is of great interest for fuel injector design, because of the need for mixing and combustion of the reactants in minimum combustor length. Important features of the near field are: (1) regions of reverse flow (as at the base of an injector or downstream of transverse fuel jets); (2) turning of the fuel and air streams, with significant transverse pressure gradients; (3) shock waves and expansion waves (for supersonic air and/or fuel streams). It is not possible to use the boundary-layer form of the conservation equations to compute even the qualitative flow behavior near the injector. This is because the boundary-layer equations tell nothing about the three flow features named in the preceeding.

In developing the computational method and in calculating test cases, attention was directed toward a fuel injector in which the fuel jet emerged from the base of the injector. The method is not restricted to this type of injection, however. For example, transverse fuel injection into a supersonic stream could also be computed. No test cases have been computed for such a flow field as yet, however. When fuel injection is through the injector base, the flow field resembles that of the well-known base flow problem, but with the added complications of fuel injection and subsequent mixing and combustion. For this reason, the numerical method was first tested against the supersonic, laminar base flow calculations of Allen and Cheng⁵, and then against the supersonic, turbulent base flow measurements of Lewis and Chapkis¹³. Both of these cases involve homogeneous, nonreacting flows. They serve to evaluate the capability of the numerical method to compute a flow with shocks, reverse flow, and a wide variety of boundary conditions. A sketch of this flow field is shown in Figure 1.

The specific objective of the present work was to develop a finite-difference method for computing the flow in the near field of a fuel injector. The general approach was to solve the time-average conservation equations for mass, momentum, energy, species, turbulence energy, and turbulence dissipation, subject to appropriate boundary conditions. These equations were written in time-dependent form, and the steady-state solution was taken to be the solution for large time. This is usually the more convenient approach from a numerical viewpoint⁷. The turbulence transport model was that of Launder and Spalding⁸, modified for compressibility effects. The main feature of this model is that the turbulence velocity scale and length scale (macroscales) at each point are determined from modeled equations for k and ϵ . These then yield the eddy viscosity (proportional to $\rho k^2/\epsilon$) and the other turbulent transport coefficients (each proportional to eddy viscosity).

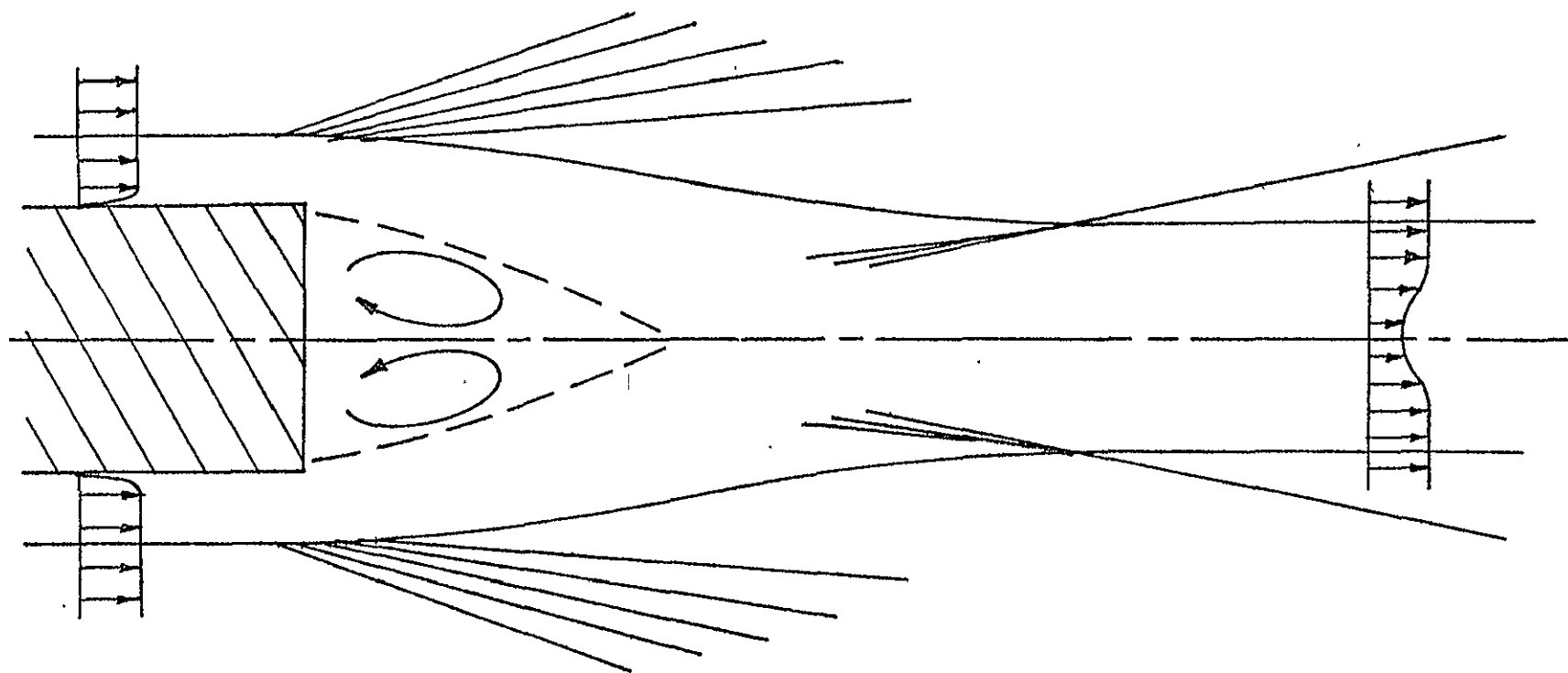


Figure 1. Sketch of flow field in the absence of base injection.

A comment may be made regarding the choice of a turbulent transport model that requires two additional partial differential equations, instead of a simpler mixing-length model. The attributes and defects of these approaches to turbulent transport modeling have been much discussed in recent years. It seems worthwhile to point out that there are some tradeoffs involved. For the mixing-length model, initial conditions are simplified, whereas initial conditions for k and ϵ are usually not available and must be guessed. On the other hand, it is difficult to specify an appropriate spatial mixing length distribution unless a great deal is already known about the flow. Finally, personal computational experience suggests that the ϵ -equation is not very well conditioned, in the sense that a poor choice of initial conditions or too coarse a grid may lead to difficulties in obtaining a numerical solution.

2.0 NUMERICAL METHOD

The numerical method used was based on that of Briley and McDonald^{9,10}. As the method is implicit in time, it offers the possibility of significant reductions in computation time to obtain a steady-state solution. In the Briley-McDonald method, backward time differencing is applied to the conservation equations. Then these equations are linearized, with respect to time level, by a Taylor series expansion about the n th time level. (Flow properties are known at the n th time level from a previous calculation). Central differences are used to replace the spatial derivatives. The result is a system of simultaneous linear algebraic equations for the flow properties at the $(n+1)$ th time level. An alternating direction implicit (ADI) technique is used to solve this system of equations.

In the present work attention has been restricted to two-dimensional plane flow. This was done because, considering the complexity of the flow, it seemed prudent to first develop the method for the simpler two-dimensional case.

Figure 2 illustrates the grid into which the flow field is subdivided and the corresponding nomenclature. The finite-difference forms of the conservation equations were derived by applying each of these equations to a control volume surrounding each grid point. This control volume is identical with the cell of dimensions $\Delta x, \Delta y$ that encloses the grid point. (See Figure 2). This approach has distinct advantages. First, it tends to force the conservation laws to be satisfied macroscopically, not only in the limit as $\Delta x, \Delta y, \Delta t$ go to zero (reference 7, p. 28). Second, it greatly aids in formulating boundary conditions, and helps assure that physically meaningful boundary conditions are applied⁵.

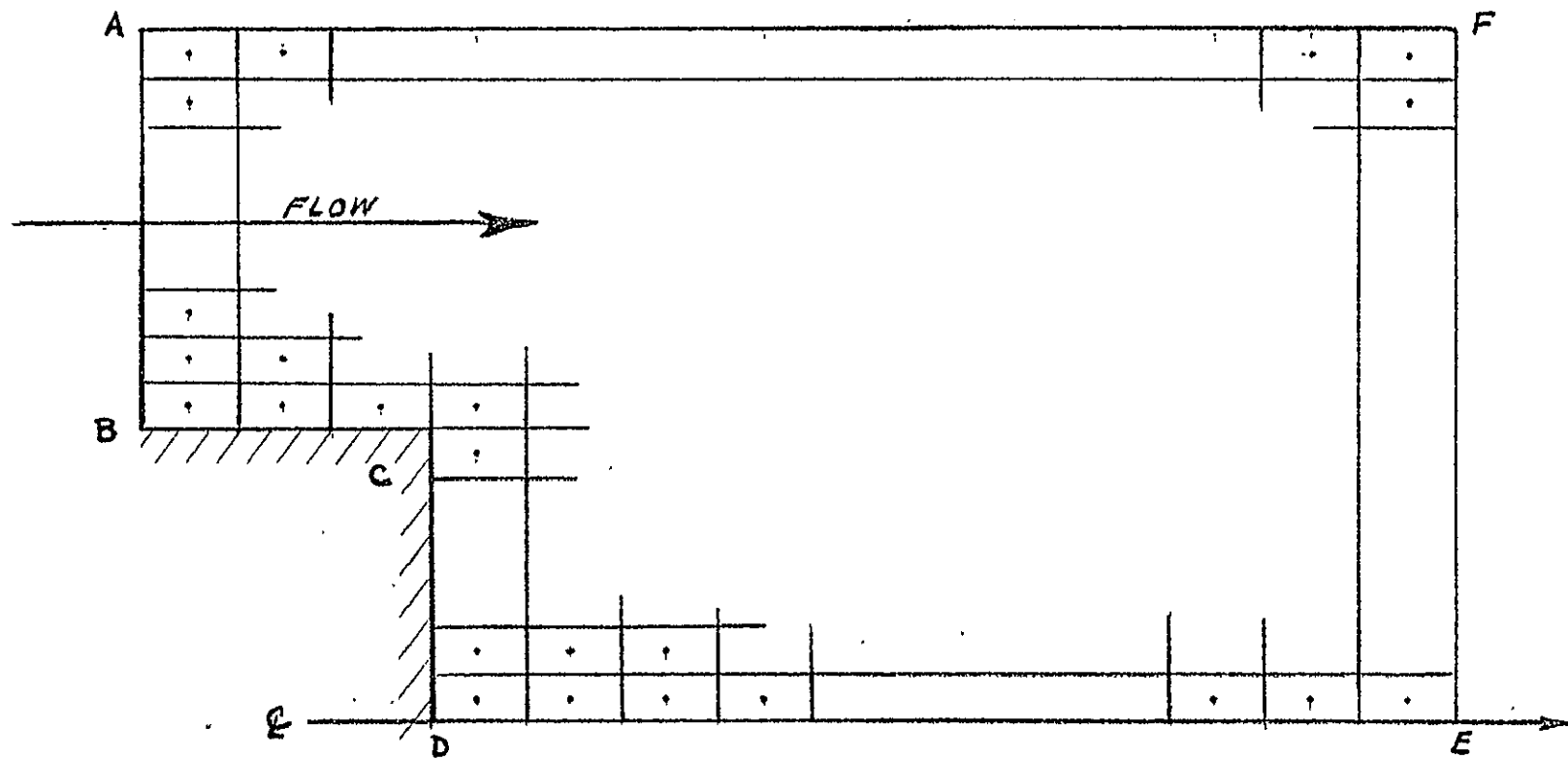


Figure 2. Flow geometry and computational field.

The derivation of the finite-difference forms of the conservation equations is given in Appendix A.

The linearization about time step n can be illustrated by considering the finite-difference equation for conservation of mass. From Appendix A, Eq. (A5), at point ij :

$$\partial \rho / \partial t = - \delta_x (\rho u) - \delta_y (\rho v) \quad (2-1)$$

Backward time-differencing is then applied to $\partial \rho / \partial t$, and the right-hand side is treated implicitly by evaluating it at the $(n+1)$ level. Eq. (2-1) then becomes:

$$(\rho^{n+1} - \rho^n)_{ij} / \Delta t = - \delta_x (\rho u)_{ij}^{n+1} - \delta_y (\rho v)_{ij}^{n+1} \quad (2-2)$$

Eq. (2-2) is nonlinear in properties at the $(n+1)$ level. So also are the remaining conservation equations after being differenced in the same way as conservation of mass. The full set of conservation equations in this finite-difference form is then a set of simultaneous nonlinear difference equations for flow properties at the $(n+1)$ level. The solution of this set of equations would require some time-consuming iterative scheme⁹.

To avoid an iterative solution, the right hand side of eq. (2-2) is linearized about the n level as follows:

$$\begin{aligned} (\rho^{n+1} - \rho^n) / \Delta t = & - \delta_x \left[(\rho u)^n + (\partial \rho u / \partial t)^n \Delta t \right] \\ & - \delta_y \left[(\rho v)^n + (\partial \rho v / \partial t)^n \Delta t \right] \end{aligned} \quad (2-3)$$

The quantity $(\partial \rho u / \partial t)^n$ is expressed in finite-difference form as:

$$(\partial \rho u / \partial t)^n = (\rho^{n+1} - \rho^n) u^n / \Delta t + \rho^n (u^{n+1} - u^n) / \Delta t \quad (2-4)$$

Using this method for $(\partial \rho v / \partial t)^n$ and collecting terms, eq. (2-3) reduces to:

$$\begin{aligned} (\rho^{n+1} - \rho^n) / \Delta t = & - \delta_x (\rho^{n+1} u^n + \rho^n u^{n+1} - \rho^n u^n) \\ & - \delta_y (\rho^{n+1} v^n + \rho^n v^{n+1} - \rho^n v^n) \end{aligned} \quad (2-5)$$

The subscript ij is to be understood in eqs. (2-3) to (2-5).

Equation (2-5) is linear in $(n+1)$ -level variables. The other conservation equations can be treated in a similar way. This set of equations could be written in the form:

$$\begin{aligned} a^n \phi_{i+1,j}^{n+1} + b^n \phi_{i,j+1}^{n+1} + c^n \phi_{ij}^{n+1} + d^n \phi_{i,j-1}^{n+1} \\ + e^n \phi_{i-1,j}^{n+1} = f^n \end{aligned} \quad (2-6)$$

Here, a^n , b^n , etc., are matrices whose order is equal to the number of dependent variables. ϕ^{n+1} is a column vector whose components are the dependent variables. f^n is a column vector containing the same number of elements as there are dependent variables.

A set of multidimensional equations such as (2-6) is usually very time consuming to solve. Considerable time savings can be realized by splitting the multidimensional equation into a series of one-dimensional equations. This was done in the present case by applying the Douglas-Gunn⁹ ADI method to each equation to obtain the intermediate steps. Each step involves implicit

solution in one of the coordinate directions. The solution of the resulting system of one-dimensional linear equations then only requires inversion of a tridiagonal matrix.

To illustrate the ADI method, consider the conservation of mass eq. (2-5). For the one-dimensional equations in the x-direction (x-sweep), (n+1)-level quantities are evaluated at an intermediate level, denoted by *. The exception is that the argument of δ_y is evaluated at the n - level. The result is:

$$(\rho^* - \rho^n)/\Delta t = -\delta_x(\rho^* u^n + \rho^n u^* - \rho^n u^n) - \delta_y(\rho^n v^n) \quad (2-7)$$

Equation (2-7) is the x-sweep part of the conservation of mass equation.

The y-sweep equation is formed from eq. (2-5) by evaluating (n+1)-level quantities at **, except for the argument of δ_x , in which (n+1)-level quantities are evaluated at *. Thus:

$$\begin{aligned} (\rho^{**} - \rho^n)/\Delta t = & -\delta_x(\rho^* u^n + \rho^n u^* - \rho^n u^n) \\ & - \delta_y(\rho^{**} v^n + \rho^n v^{**} - \rho^n v^n) \end{aligned} \quad (2-8)$$

Finally, it is convenient to subtract eq. (2-7) from eq. (2-8) and use the result as the y-sweep equation. This is:

$$(\rho^{**} - \rho^*)/\Delta t = -\delta_y(\rho^{**} v^n + \rho^n v^{**} - 2\rho^n v^n) \quad (2-9)$$

Quantities denoted by the superscript * are intermediate results obtained from the solution of the set of one-dimensional (x-direction) equations of which eq. (2-7) is a member. The other equations in this set are formed

from the other conservation equations in a manner similar to that of eq. (2-7). Likewise, each of the conservation equations is used to form y-sweep equations corresponding to eqs. (2-8) and (2-9). The use of eq. (2-9) instead of eq. (2-8) halves the storage requirement and reduces the computational effort. It has been shown⁹ that ϕ^{**} is within order $(\Delta t)^2$ of ϕ^{n+1} , and so is taken as ϕ^{n+1} . The complete set of x-sweep and y-sweep equations is given in Appendix B.

The finite-difference forms of the conservation equations, such as eqs. (2-7) and (2-9), can be written in the following general form:

$$c_i^n \phi_{i-1,j}^* + b_i^n \phi_{ij}^* + a_i^n \phi_{i+1,j}^* = d_i^n \quad (2-10)$$

$$\gamma_j^n \phi_{i,j-1}^{**} + \beta_j^n \phi_{ij}^{**} + \alpha_j^n \phi_{i,j+1}^{**} = \xi_j^* + \eta_j^n \quad (2-11)$$

Here c , b , a , γ , β , and α are two-dimensional matrices. ϕ is the dependent variable column matrix, and d , ξ , and η are column matrices.

The solution procedure for a single time step is as follows. First, eq. (2-10) is applied to successive rows (x-direction) to generate a set of coupled, one-dimensional equations. These implicit equations are arranged into a block tridiagonal matrix for each row, and solved for ϕ^* by a standard elimination technique. Second, eq. (2-11) is applied to successive columns (y-direction). Following the same procedure, ϕ^{**} is computed at each grid point.

The technique used to solve these equations is the LU decomposition and back-substitution (LUBS) method of Isaacson and Keller¹¹. A discussion of the application of this method to the present problem is given in reference 3.

3.0 BOUNDARY CONDITIONS

The finite-difference equations have the same form for each of the interior grid points. These equations must be modified for cells which are adjacent to the boundaries of the computational field, however, to properly represent the physical boundary conditions. The particular boundary conditions are described here relative to the injector flow field sketch in Figure 2.

3.1. Upper Wall (BC)

Consider the cell with grid point ij adjacent to wall BC. (See Figure 3). Because this is an impermeable wall,

$$(v)_{y-} = 0 \quad (3-1)$$

Also, to satisfy the no-slip condition,

$$(u)_{y-} = 0 \quad (3-2)$$

In the x-momentum equation, the nondimensional shear stress at the wall is

$$\left[(\mu_T + \mu/R_1) s_{xy} \right]_{y-} \cdot \text{Thus,} \quad (3-3)$$

$$\left[(\mu_T + \mu/R_1) s_{xy} \right]_{y-} = \rho_{ij} u_*^2$$

and u_* is calculated from the Law of the Wall for a smooth wall:

$$u_{ij}/u_* = (1/\kappa) \ln \left[(\rho y/\mu)_{ij} u_* R_1 \right] + 5 \quad (3-4)$$

In applying (3-4), care was taken that $(\rho y/\mu)_{ij} u_* R_1 > 30$. It was also assumed that eq. (3-4) was valid between $(y-)$ and $(y+)$. Then, $\partial u/\partial y = u_*/\kappa y$. This provided a method of treating the shear stress terms in the y-momentum equation. Thus,

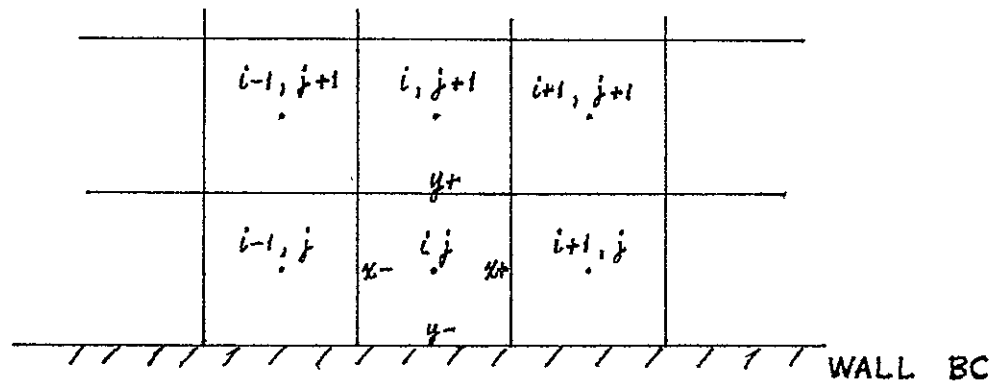


Figure 3. Cell adjacent to wall BC.

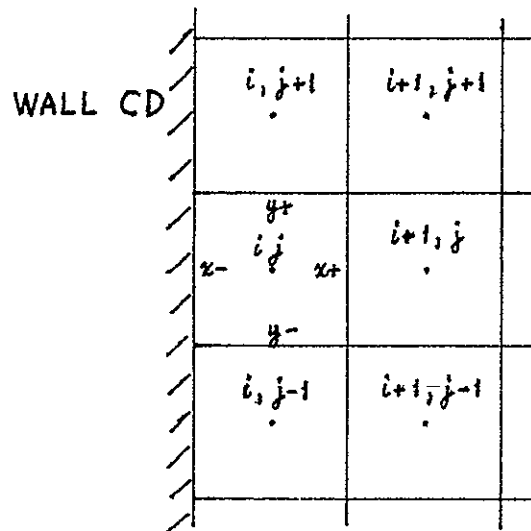


Figure 4. Cell adjacent to wall CD.

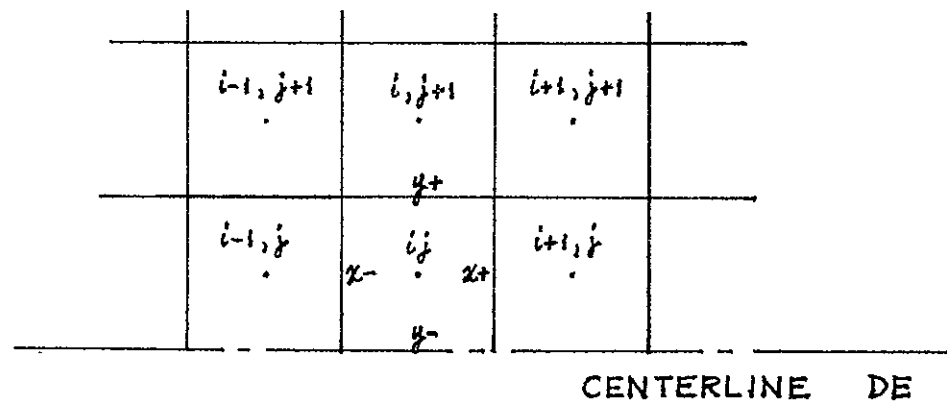


Figure 5. Cell adjacent to centerline DE.

$$\left[(\mu_T + \mu/R_1) s_{xy} \right]_{x^+} = \left[(\mu_T + \mu/R_1) \partial v / \partial x \right]_{x^+} + (\rho u_*^2)_{x^+} \quad (3-5)$$

and similarly for $\left[(\mu_T + \mu/R_1) s_{xy} \right]_{x^-}$.

The nondimensional pressure at the wall is equal to $(\rho e)_{y^-}$. This quantity was evaluated by a linear extrapolation through (ij) and $(i,j+1)$, so that,

$$(\rho e)_{y^-} = 1.5 (\rho e)_{ij} - 0.5 (\rho e)_{i,j+1} \quad (3-6)$$

Because of eq. (3-2), it was also required that,

$$(\partial u / \partial x)_{y^-} = 0 \quad (3-7)$$

Normal derivatives at a surface were represented by a second-order accurate, one-sided difference approximation⁵:

$$(\partial \phi / \partial y)_{y^-} = (-8 \phi_{y^-} + 9 \phi_{ij} - \phi_{i,j+1}) / 3 \Delta y \quad (3-8)$$

This gives: $(\partial v / \partial y)_{y^-} = (9 v_{ij} - v_{i,j+1}) / 3 \Delta y \quad (3-9)$

Because turbulent velocity fluctuations go to zero at a solid boundary, it was required that,

$$(\mu_T)_{y^-} = 0 \quad (3-10)$$

and,

$$(k)_{y^-} = 0 \quad (3-11)$$

Following the approach used in eq. (3-5), the condition,

$$\left[(\mu_T + \mu/R_1) (\partial u / \partial y) \right]_{x+} = (\rho u_*^2)_{x+} \quad (3-12)$$

was imposed, and similarly for the value at $x-$.

For the present calculations, it was assumed that the wall was adiabatic. Then,

$$(q_y)_{y-} = - (\partial e / \partial y)_{y-} = 0 \quad (3-13)$$

It was assumed that there is no variation in composition normal to the wall at the wall. Thus,

$$(\partial C_a / \partial y)_{y-} = 0 \quad (3-14)$$

The Law of the Wall was also used to determine certain quantities at (ij). Thus,

$$(\partial u / \partial y)_{ij} = \overline{u_* / \nu} y_{ij} \quad (3-15)$$

$$k_{ij} = u_*^2 / C_\mu^{0.5} \quad (3-16)$$

$$\epsilon_{ij} = u_*^3 / \nu y_{ij} \quad (3-17)$$

3.2 Back Wall (CD)

Now consider the cell with grid point (ij) whose ($x-$) edge coincides with the back wall. (See Figure 4).

For an impermeable wall,

$$(u)_{x-} = 0 \quad (3-18)$$

and for no slip at the wall,

$$(v)_{x-} = 0 \quad (3-19)$$

Also from eqs. (3-18) and (3-19):

$$(\partial u / \partial y)_{x-} = 0 \quad (3-20)$$

$$(\partial v / \partial y)_{x-} = 0 \quad (3-21)$$

Using eq. (3-8) for normal derivatives at the wall gives:

$$(\partial u / \partial x)_{x-} = (9 u_{ij} - u_{i+1,j}) / 3 \Delta x \quad (3-22)$$

and

$$(\partial v / \partial x)_{x-} = (9 v_{ij} - v_{i+1,j}) / 3 \Delta x \quad (3-23)$$

The pressure at the back wall was obtained in the same way as on the upper wall by eq. (3-6).

$$(pe)_{x-} = 1.5(pe)_{ij} - 0.5(pe)_{i+1,j} \quad (3-24)$$

For an adiabatic wall,

$$(q_x)_{x-} = - (\partial e / \partial x)_{x-} = 0 \quad (3-25)$$

Because of eqs. (3-18) and (3-19), the shear-work terms are zero:

$$(s_{ix} u_i)_{x-} = 0 \quad (3-26)$$

At the wall, the turbulent velocity fluctuations are zero. Thus

$$(k)_{x-} = 0 \quad (3-27)$$

and,

$$(\mu_T)_{x-} = 0 \quad (3-28)$$

Also, similar to eq. (3-14), the assumption was made that,

$$(\partial C_a / \partial x)_{x-} = 0 \quad (3-20)$$

3.3 Centerline (DE)

Because DE is a plane of symmetry, there is no mass flux across it.

Figure 5 shows a typical cell adjacent to DE.

$$(v)_{y-} = 0 \quad (3-30)$$

This also gives,

$$(\partial v / \partial x)_{y-} = 0 \quad (3-31)$$

and,

$$(\partial v / \partial y)_{y-} = (9v_{ij} - v_{i,j+1}) / 3\Delta y$$

Also because of symmetry,

$$(\partial \phi / \partial y)_{y-} = 0 \quad (3-32)$$

Combining eq. (3-32) with eq. (3-8) gives a formula for any dependent variable except v at $(y-)$:

$$\phi_{y-} = (9/8)\phi_{ij} - (1/8)\phi_{i,j+1} \quad (3-33)$$

Equations (3-30) through (3-32) also give:

$$(s_{iy} u_i)_{y-} = 0 \quad (3-34)$$

3.4 Outflow Boundary (EF)

For this case the x^+ cell boundary is located along EF. The approach followed here was the same as that recommended by Roache (reference 7, pp. 279-281). Properties at (ij) are determined by a linear extrapolation

through (i-1,j) and (i-2,j), giving:

$$\phi_{ij} = 2\phi_{i-1,j} - \phi_{i-2,j} \quad (3-35)$$

3.5 Upper Boundary (AF)

The cell with grid point (ij) has its y+ edge along AF. Flow properties at (ij) were determined by considering the straight left-running characteristic that passes through (ij). Properties are approximately constant along this characteristic, and can be determined by suitable interpolation from the properties at (i-1,j-1) and (i,j-1), or (i-1,j-1) and (i-1,j). The procedure is described by Roache (reference 7, pp. 282-283). Referring to Figure 6a, when $\tan(\mu_M + \theta)_{i-1,j-1} > \Delta y/\Delta x$, then:

$$\phi_p = \phi_{i-1,j-1} + (\ell/\Delta x)(\phi_{i,j-1} - \phi_{i-1,j-1}) \quad (3-36)$$

By this approximation, $\phi_p = \phi_{ij}$. Next, let

$$w'_p = \tan \left[90^\circ - (\mu_M + \theta)_p \right]$$

Now, $w'_p = (\Delta x - \ell)/\Delta y$ by geometry. An expression for w'_p can also be obtained from eq. (3-36). Equating these two and solving for ℓ gives,

$$\ell = (\Delta x/\Delta y - w'_{i-1,j-1}) / \left[(w'_{i,j-1} - w'_{i-1,j-1}) / \Delta x + 1/\Delta y \right] \quad (3-37)$$

when $\tan(\mu_M + \theta)_{i-1,j-1} > \Delta y/\Delta x$.

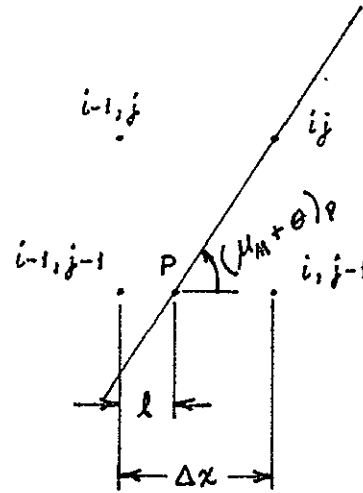


Figure 6a. Upper boundary AF. $\tan (\mu_M + \theta)_{i-1,j-1} > \Delta y / \Delta x$.

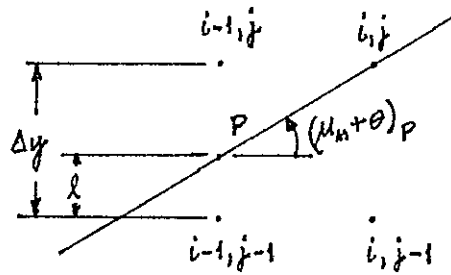


Figure 6b. Upper boundary AF. $\tan (\mu_M + \theta)_{i-1,j-1} < \Delta y / \Delta x$.

Next, consider Figure 6b, which depicts the case when $\tan (\mu_M + \theta)_{i-1,j-1} < \Delta y / \Delta x$. Let,

$$w_p = \tan (\mu_M + \theta)_p$$

For constant properties along a left-running characteristic,

$$\phi_p = \phi_{i-1,j-1} + (\ell / \Delta y)(\phi_{i-1,j} - \phi_{i-1,j-1}) \quad (3-38)$$

Also, by geometry, $w_p = (\Delta y - \ell) / \Delta x$. As before, these relationships yield a formula for ℓ :

$$\ell = (\Delta y / \Delta x - w_{i-1,j-1}) / \left[(w_{i-1,j} - w_{i-1,j-1}) / \Delta y + 1 / \Delta x \right] \quad (3-39)$$

for $\tan (\mu_M + \theta)_{i-1,j-1} < \Delta y / \Delta x$.

Equations (3-37) and (3-39) are then used in eqs. (3-36) and (3-38), respectively, to compute the remaining properties at p .

3.6 Inflow Boundary (AB)

Flow properties at the inflow boundaries were specified and kept fixed as the solution developed in time.

4.0 RESULTS

In this section some results of computations using the present numerical method are given. Two sets of calculations are described. The first is for a supersonic, laminar base flow at conditions previously computed by Allen and Cheng⁵. The second is for a supersonic, turbulent base flow at the conditions of the experiments of Lewis and Chapkis.¹²

The laminar flow case is simpler, as it involves fewer differential equations (four). These laminar flow calculations have been very important to the program development, because they have served to establish effects of variations in boundary conditions, grid size, time step, and other parameters, without the additional complications of turbulent flow. Some of this work is still continuing, as indicated in what follows. These calculations have also served to establish that the numerical method is stable and convergent.

The laminar flow calculations were made for $M_1 = 3$, $R_1 = 550$, and nondimensional initial boundary-layer thickness $\delta = 0.41$. The initial u -profile was the polynomial in y used by Allen and Cheng. The corresponding v was obtained from the continuity and x -momentum boundary-layer equations.⁵ e was given by the Busemann integral for an adiabatic wall, and p was uniform and equal to its freestream value. The computational mesh size was $\Delta x = 1/6$ and $\Delta y = 1/12$. This is coarser than that used by Allen and Cheng, and was chosen to increase economy while retaining reasonable accuracy during program development. The computational time step used was four times the Courant-Friedricks-Lewy (CFL) time step, which is the maximum time step for stable calculation using an explicit, finite-difference method. Stable and convergent solutions were obtained with the larger time step using the present implicit method, thus demonstrating potentially large savings in computer time.

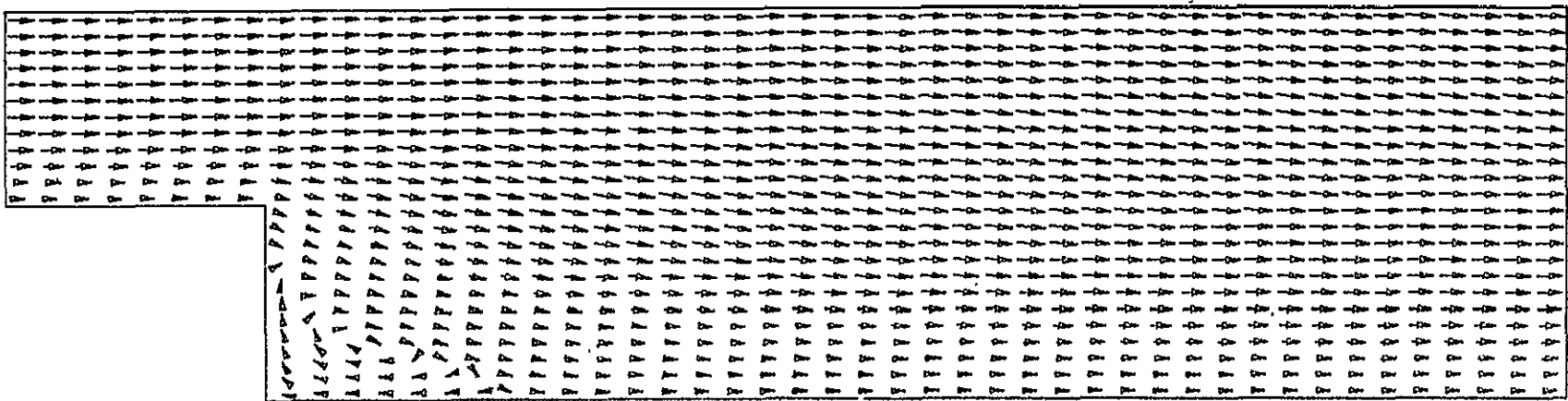
Figures 7 - 13 show computed results for the laminar flow case

described in the preceding. Figure 7 shows the field of velocity vectors. All the main features of the flow are evident here, including the initial boundary layer, the expansion and turning at the corner, the weak recompression shock and turning downstream, the recirculation region near the base, and the retarded flow near the plane of symmetry. The location of the rear stagnation point is about 20% closer to the base than that calculated by Allen and Cheng.⁵ The dividing streamline separates just below the corner, in agreement with previous experiments and calculations.⁵

The streamline plot of Figure 8 shows the flow turning due to expansion and recompression even more clearly. Also, the recirculation region and the dividing streamline are indicated. The pressure contours of Figure 9 very effectively illustrate the corner expansion and the recompression shock. Also note that downstream of the recirculation region there is a growing region where $\partial p / \partial y \approx 0$ near the plane of symmetry. Results of this kind indicate the region of validity of the boundary-layer equations, which are usually used to describe the wake at some distance from the body. The density contours of Figure 10 also show the expansion and recompression. For the case of an adiabatic wall, the density near the wall is less than the free-stream value, and this is indicated in the solution. Corresponding internal energy contours are shown in Figure 11.

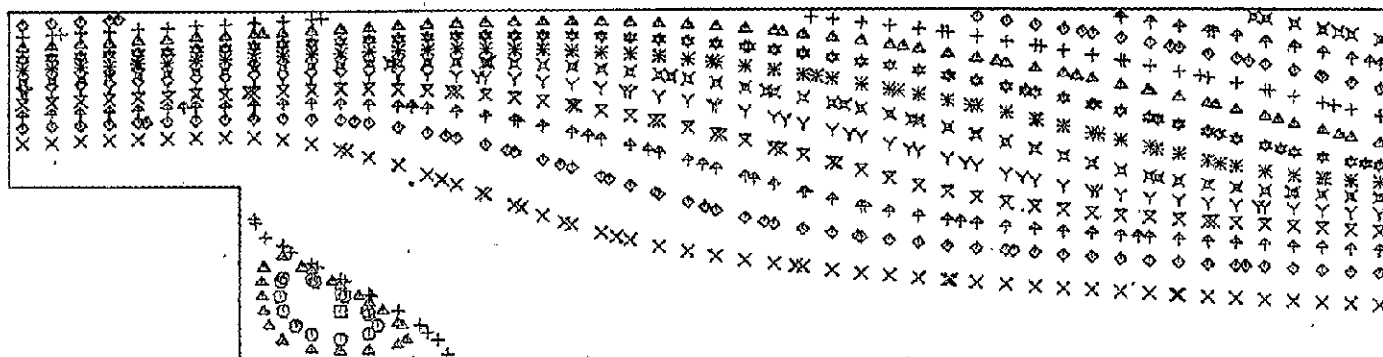
The computed centerline pressure distribution is given in Figure 12. Also shown are the calculated results of Allen and Cheng.⁵ The two are in close agreement.

Centerline Mach number distribution is shown in Figure 13. This figure illustrates the extent of the recirculation region and the acceleration of the flow in the downstream direction. Downstream of the region of the present computation, the centerline Mach number will exceed one. A short



VELOCITY VECTORS

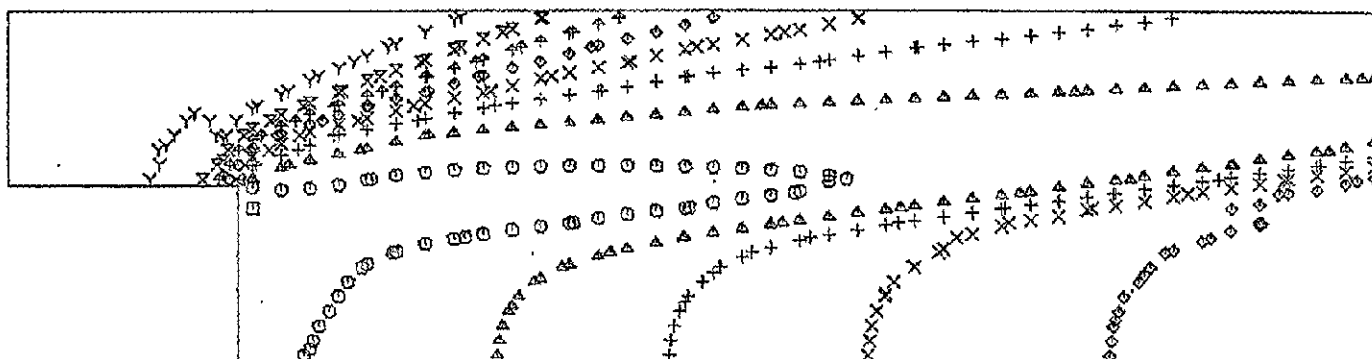
Figure 7. Velocity vectors. Laminar flow.



STREAMLINES

Figure 8. Streamlines. Laminar flow.

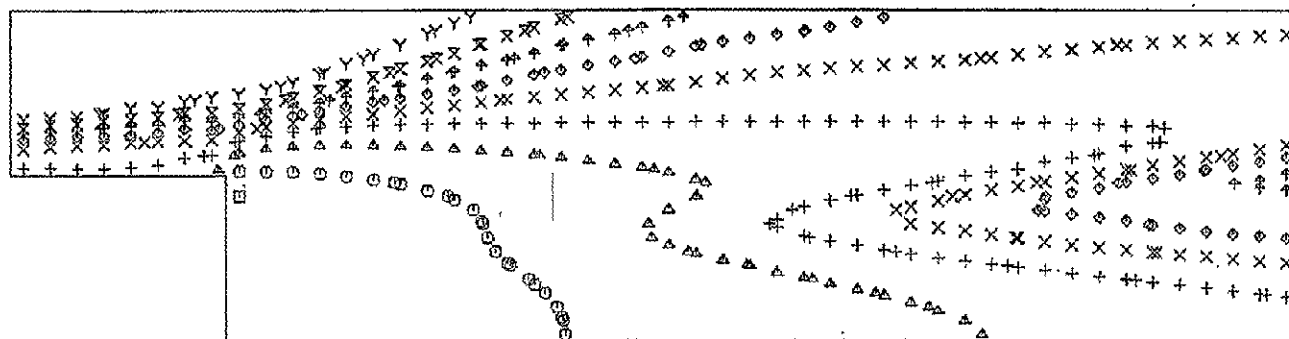
□	○	△	+	X	◇	+	X	Y	X
0.091	0.195	0.299	0.403	0.506	0.610	0.714	0.818	0.922	1.026



PRESSURE CONTOURS

Figure 9. Pressure contours. Laminar flow.

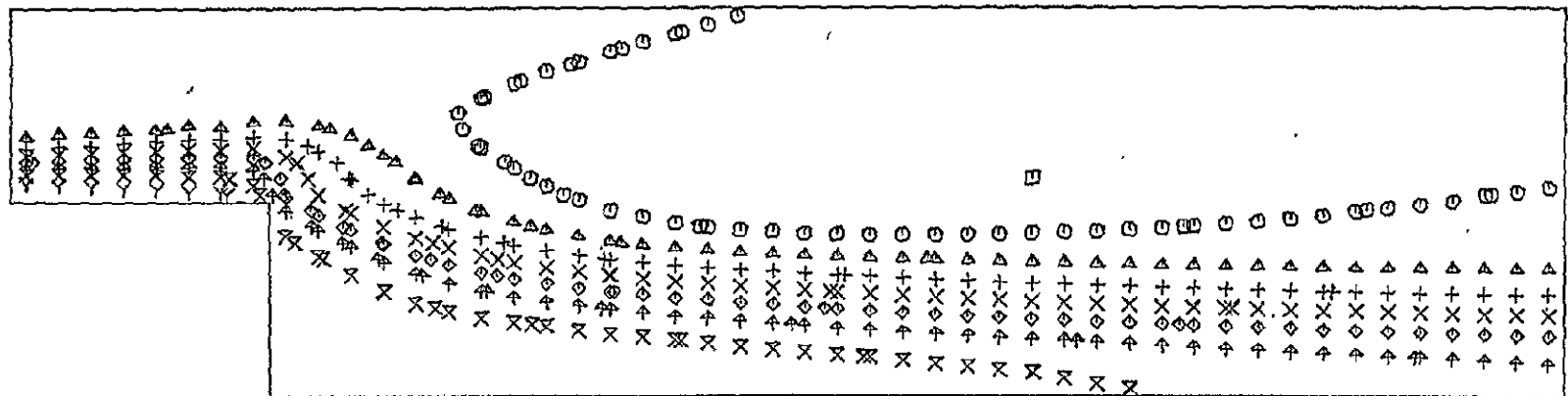
□	⊙	△	+	×	◇	†	⌘	Y	⌘
0.041	0.149	0.258	0.367	0.476	0.585	0.693	0.802	0.911	1.020



DENSITY CONTOURS

Figure 10. Density contours. Laminar flow.

□	○	△	+	X	◇	⋈	⊗	Y	⊗
0.657	0.890	1.123	1.356	1.589	1.822	2.056	2.289	2.522	2.755



INTERNAL ENERGY CONTOURS

Figure 11. Internal energy contours. Laminar flow.

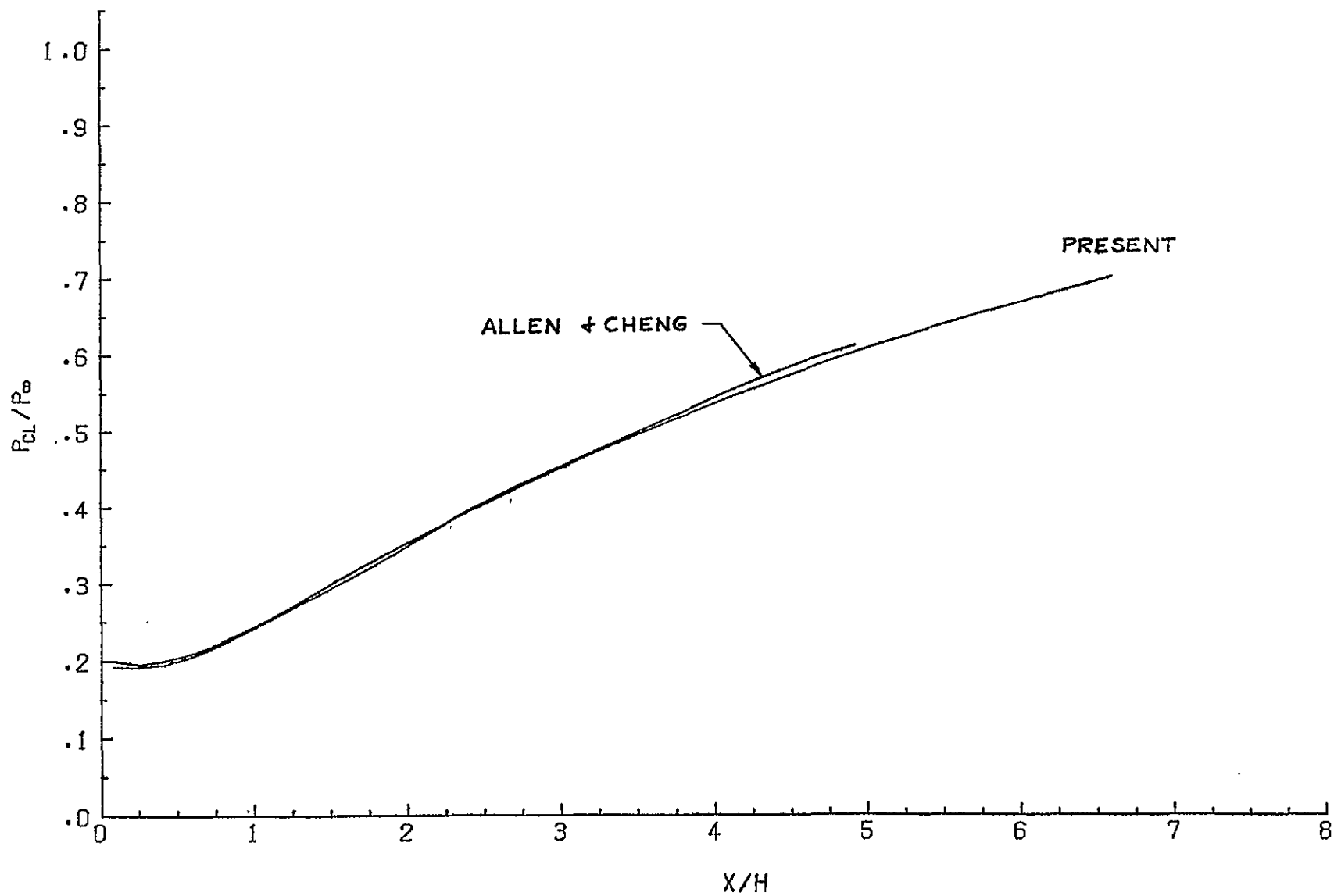


Figure 12. Centerline pressure distribution. Laminar flow.

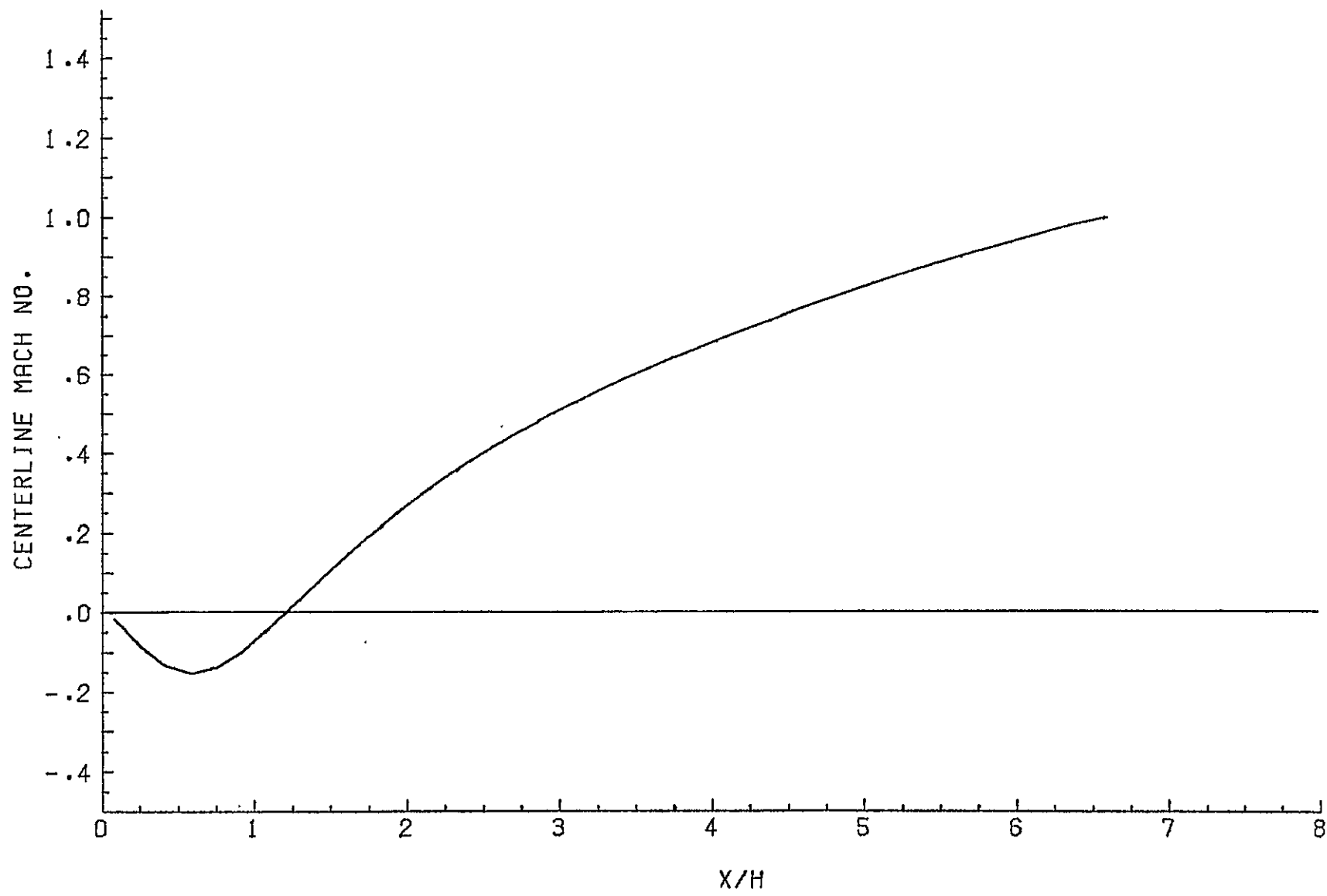


Figure 13. Centerline Mach number distribution. Laminar flow.

distance away from the centerline at the outflow boundary, the flow is already supersonic. It is perhaps worth noting that there is no singularity encountered, such as the Crocco-Lees singularity, associated with the Mach one condition.

Information concerning the convergence and the computation time of the present method is given in Figure 14. To evaluate the degree of convergence of the solution, the fractional change in each variable between successive time steps is evaluated at each grid point. The maximum fractional change for each variable and its location are then printed for each time step. Experience with the present method indicates that the density variation is a sensitive measure of convergence. Of course, by examining the changes in all the variables, as is being done, larger variations in some other variable can be easily detected. Figure 14 shows the fractional change in density plotted against number of time steps and against total computation time. Up to step 110, the maximum density change shown occurred on the centerline at the downstream boundary. Starting with step 111, the maximum change occurred on the back wall at about 0.6 H from the centerline. The maximum change remained close to the back wall for the rest of the computation. At step 450 the computation was stopped when the maximum fractional change in density had fallen to 0.0001.

The computational time step was four times the CFL time step. This value was chosen arbitrarily, as being significantly larger than the explicit stability limit, yet not so large as to cause excessive problems related to the choice of initial conditions. Briley and McDonald^{9,10} used much larger time steps, but confined their attention to a much simpler flow. It is believed that the present results provide a significant demonstration of the basic stability and convergence of the method. Other tests, including the

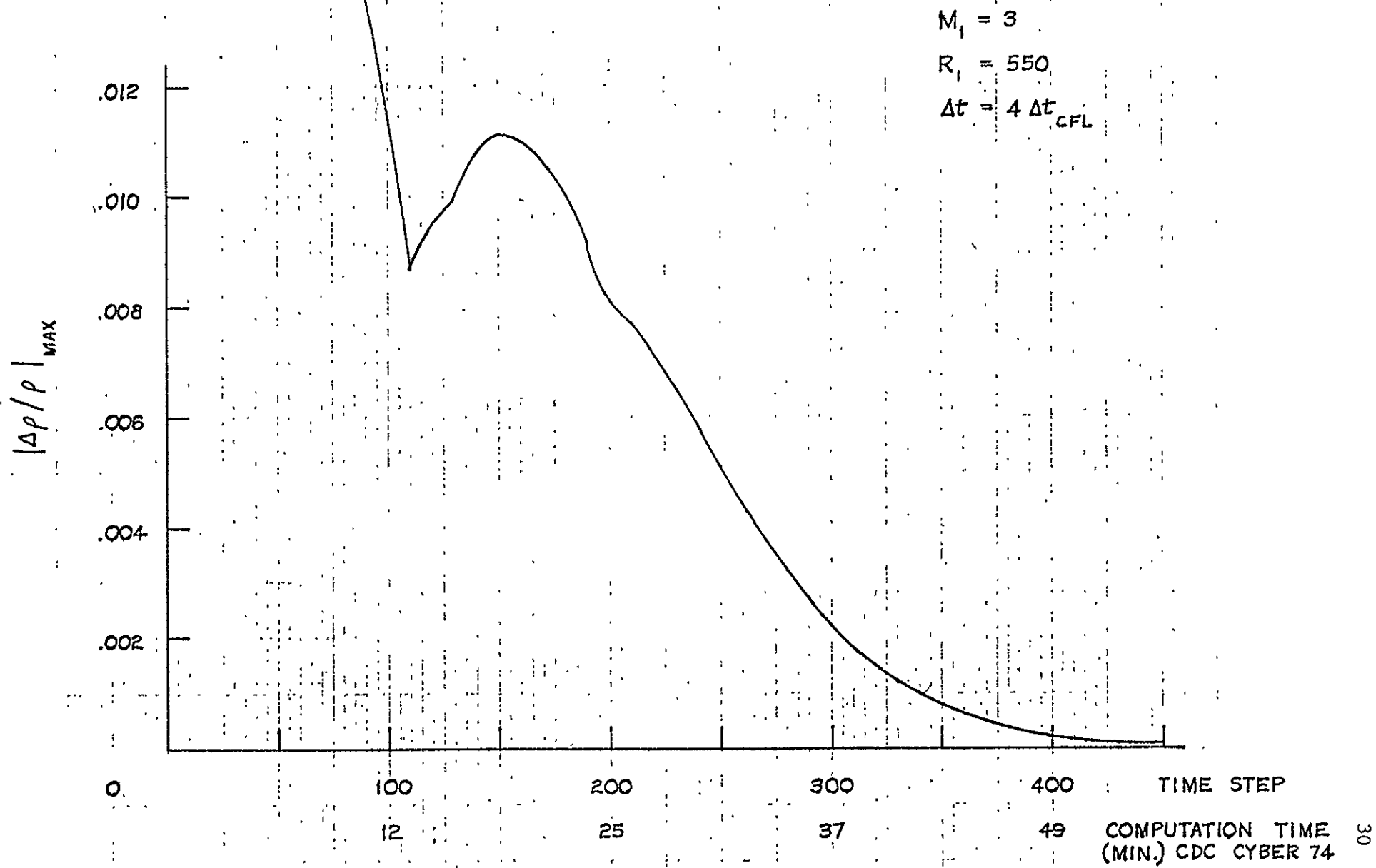


Figure 14. Variation of maximum fractional change in density. Laminar flow.

use of widely varying initial conditions and different time step sizes, must be performed in order to develop a more complete picture of the behavior of the method. This work is still being performed. The present computations had initial ρ and e equal to freestream values everywhere except in the inflow boundary layer. For $y > H$, $u = 1$ (freestream velocity) except in the inflow boundary layer, and for $y < H$, $u = 0.3$. Finally, $v = 0$ everywhere initially, except in the inflow boundary layer.

The net mass flux through the field of computation was also monitored in these calculations. In the steady state, the net mass flux should be zero. At time step 450, where the calculations were halted, the total inflow differed from the total outflow by 1.8%.

It seems significant that while conditions near the expansion corner converged most slowly, the remainder of the flow was almost unchanged after about time step 100. In a complex flow such as this, with a number of different length scales and velocity scales, different parts of the flow will converge to the steady state at different rates. Thus, it may be possible to shorten the calculation in cases where the most slowly converging portion is not of primary interest.

The potential advantages in computation time of using even larger time steps have not yet been explored. This is now being done, as reduced computation time is probably the most attractive feature of the present numerical method. In this connection, the second abscissa of Figure 14 is of interest. Here the computation (CPU) time is indicated. For laminar flow, the method takes about 7 milliseconds per grid point per time step on a CDC-CYBER 74 machine. The present grid has 1056 points. These computation times seem promising, especially if significantly larger time steps can be taken.

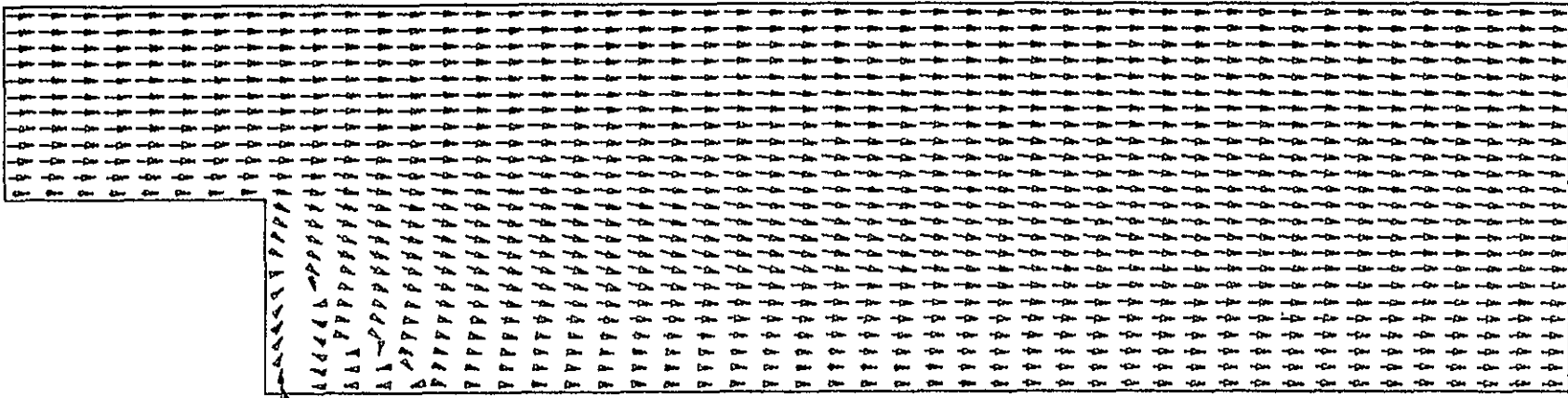
A calculation of a supersonic, two-dimensional, turbulent base flow

was made at the conditions of the experiments of Lewis and Chapkis.¹² These were $M_1 = 4.0$, $R_1 = 162,000$, and $\delta = 0.31$. The initial u -profile in the boundary layer at AB was a power-law profile with exponent $1/3.7$. v was zero. ϵ was given by the Busemann integral for an adiabatic wall.⁵ The pressure was uniform and equal to the freestream value. As before, $\Delta x = 1/6$ and $\Delta y = 1/12$. The time step was again four times the CFL value. In this case, however, the k and ϵ equations were solved to give $\mu_T = C_\mu \rho k^2 / \epsilon$.

In the experiments¹², the expansion corner was preceded by a 6° half-angle wedge. This precompression was omitted from the present calculations for simplicity, so that the inflow would be parallel to x . Thus, the 2% loss in stagnation pressure across the bow shock was not simulated.

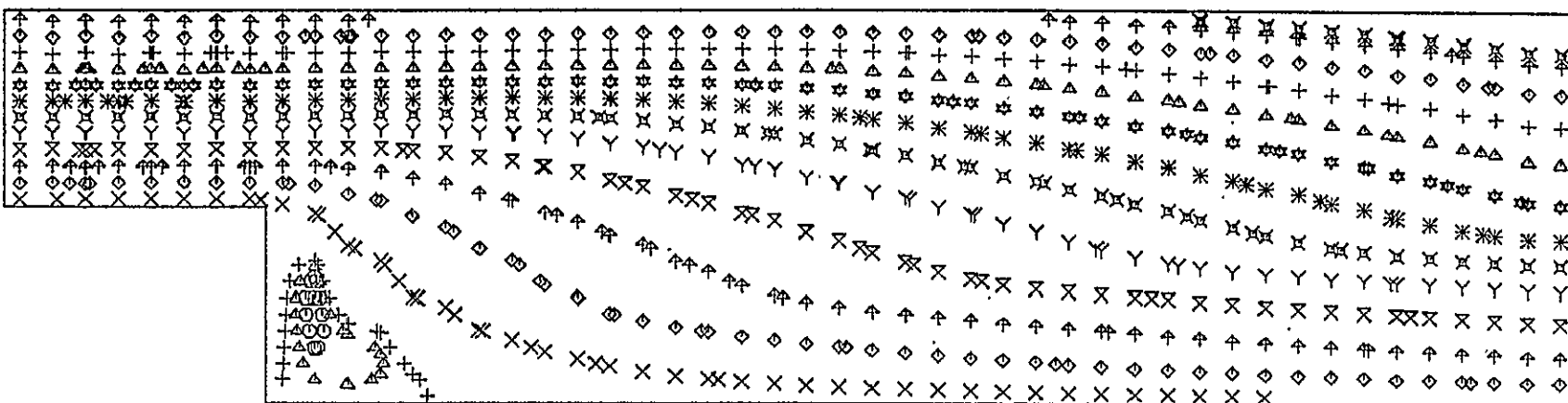
Figure 15 shows the field of mean velocity vectors for this turbulent flow case. All the qualitative features of the flow are present, including the initial boundary layer, the turning by the corner expansion, the turning by the recompression shock, the recirculation near the base, and the retarded viscous wake. The streamlines are shown in Figure 16. Again the flow turning because of expansion, recompression, and recirculation is evident. The streamline spacing increases during expansion and decreases during compression. The extent of the recirculation region is too small, however, compared with the experimental data. Also, the dividing streamline is not clearly shown. This may be partly due to the pressure wiggles that appear in Figures 17 and 22.

Figures 17, 18, and 19 show the contours of pressure, density, and internal energy, respectively. These all show the correct qualitative behavior, in that the expansion, recompression shock, and recirculation are clearly shown. Figures 20 and 21 show the k and ϵ contours, respectively. The numerical values on the figures are one hundred times the



VELOCITY VECTORS

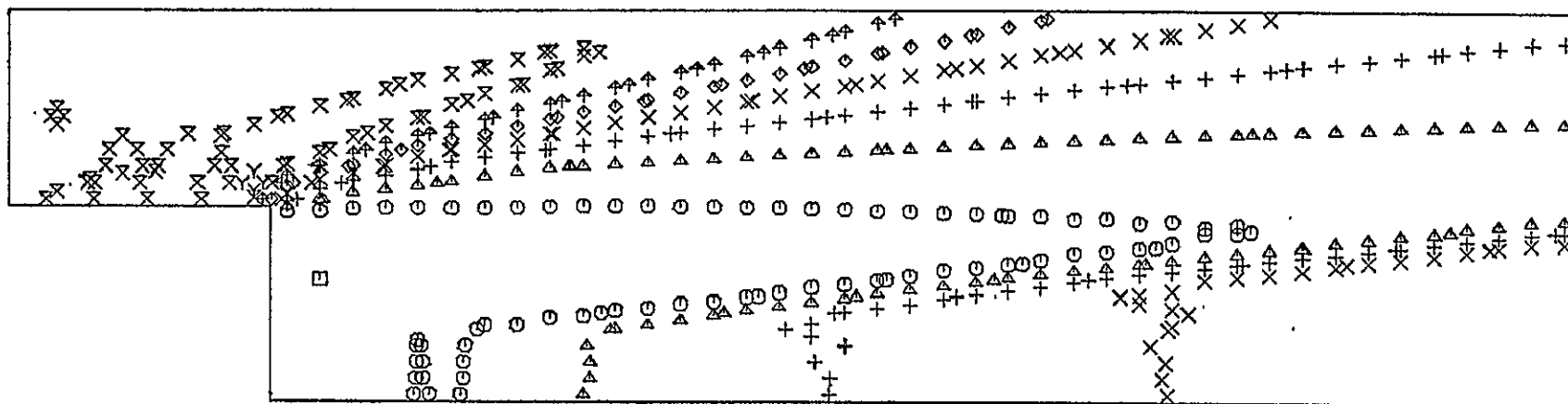
Figure 15. Velocity vectors. Turbulent flow.



STREAMLINES

Figure 16. Streamlines. Turbulent flow.

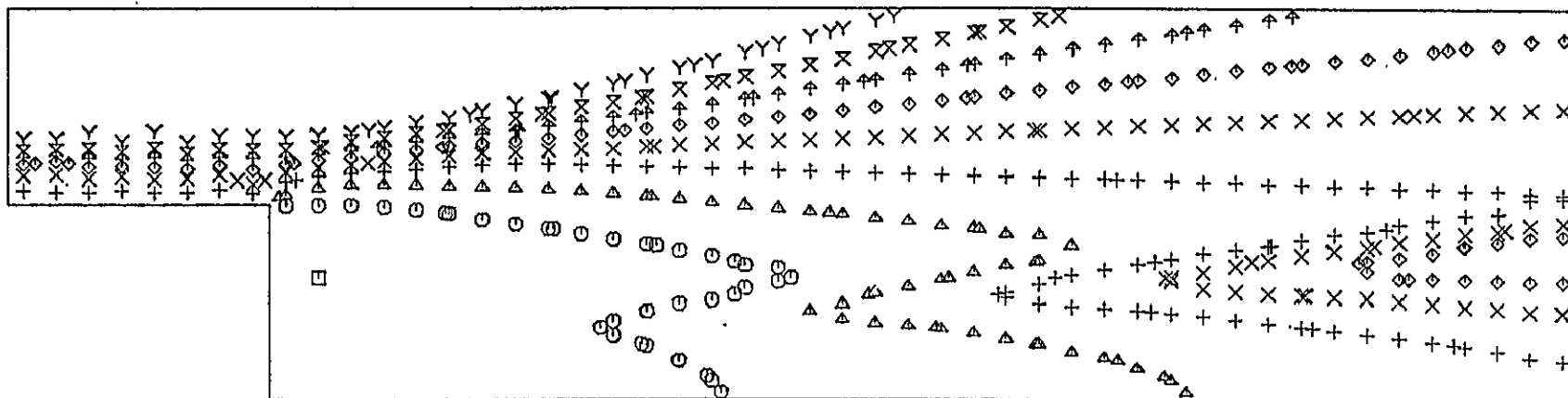
□	○	△	+	×	◇	⬆	⋈	Y	✕
0.054	0.201	0.347	0.493	0.639	0.786	0.932	1.078	1.224	1.370



PRESSURE CONTOURS .

Figure 17. Pressure contours. Turbulent flow.

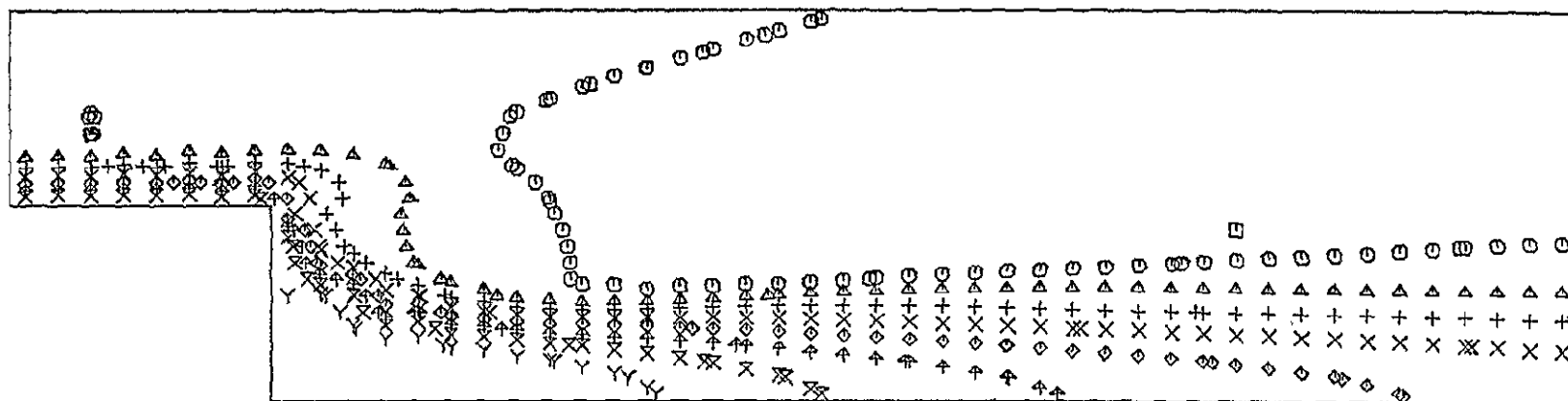
□	○	△	+	X	◇	⤴	⌘	Y	⌘
0.019	0.136	0.252	0.369	0.486	0.603	0.719	0.836	0.953	1.070



DENSITY CONTOURS

Figure 18. Density contours. Turbulent flow.

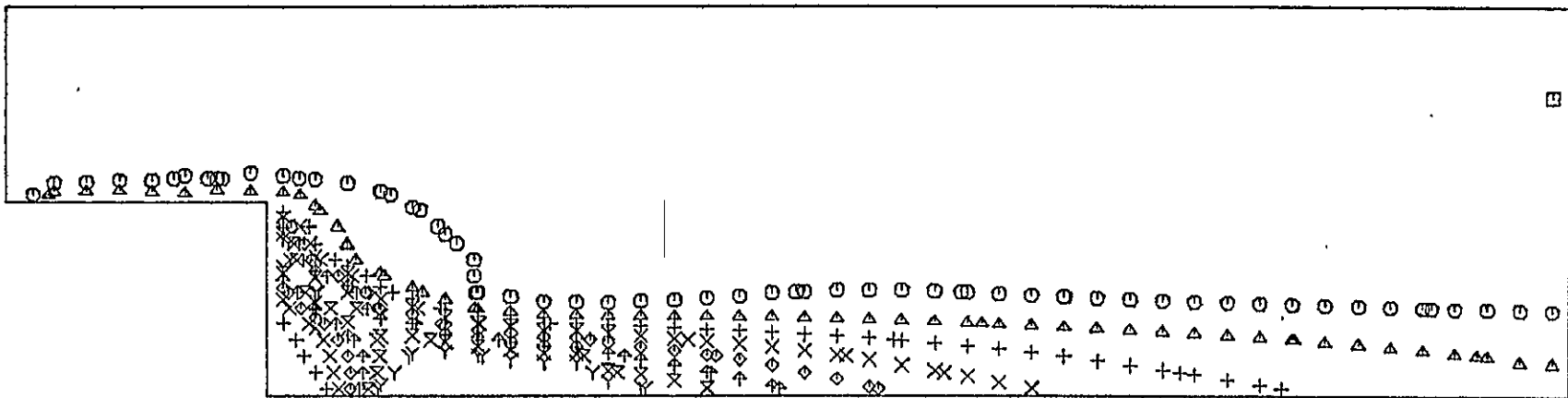
□	○	△	+	×	◇	↑	×	Y	×
0.655	0.999	1.343	1.686	2.030	2.374	2.717	3.061	3.405	3.748



INTERNAL ENERGY CONTOURS

Figure 19. Internal energy contours. Turbulent flow.

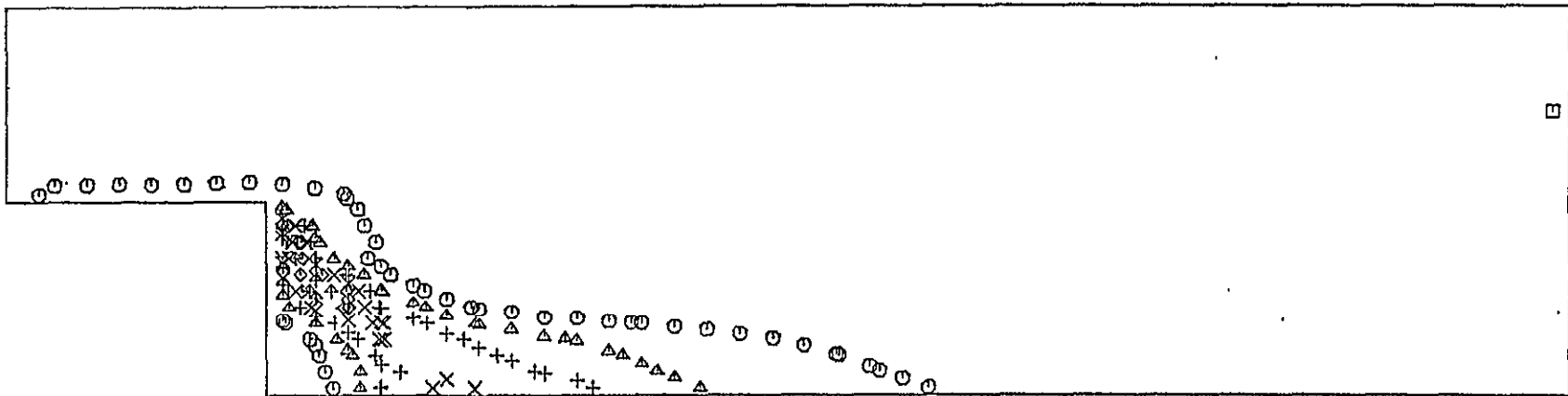
□	○	△	+	×	◇	↑	✕	Y	✕
0.216	1.303	2.390	3.477	4.564	5.652	6.739	7.826	8.913	10.000



TURBULENCE KINETIC ENERGY CONTOURS

Figure 20. Turbulence kinetic energy contours.

□	○	△	+	×	◇	⬆	⋈	Y	⋈
0.021	1.326	2.631	3.936	5.241	6.545	7.850	9.155	10.460	11.765



DISSIPATION RATE CONTOURS

Figure 21. Turbulence dissipation rate contours.

computed values. k and ϵ take on their largest values where the shear stresses are largest.

The centerline pressure distribution is shown in Figure 22, along with the data of Lewis and Chapkis.¹² The calculation is fairly consistent with the experimental data, except that it does not show the sharp rise in pressure near $x/H = 2$. This result, plus the smaller computed recirculation region, may be caused by the turbulence model. The effect of the turbulence model on mean flow properties such as these would seem to be a useful area for further research.

Figure 23 shows the corresponding Mach number distribution.

Figure 24 is a plot of $|\Delta\rho/\rho|_{\max}$ versus time step, showing the approach of the solution to convergence. The flow field was virtually unchanged after step 150. Between steps 156 and 254, $|\Delta\rho/\rho|_{\max}$ occurred close to the back wall, about halfway up. From steps 255 to 300, the location shifted among four places in or near the recirculation region. The calculation was stopped at step 300 where $|\Delta\rho/\rho|_{\max} = 0.0002$. Also, at this step the net mass inflow differed from the net mass outflow by 2.3%.

Careful examination of the calculations makes it clear that the pressure wiggles originate at the outflow boundary near the recompression shock. Similar behavior was previously encountered with the laminar flow calculations, when the condition $\partial\phi/\partial x = 0$ was imposed along EF. This condition, when combined with either a linear or a quadratic variation of $\phi(x)$, produced wiggles that had their largest amplitude near the back wall. Use of equation (3-35) eliminated the wiggles for the laminar flow case. Further study of the outflow boundary condition is needed, in particular to determine whether the turbulence model has any effect on the appearance of wiggles.

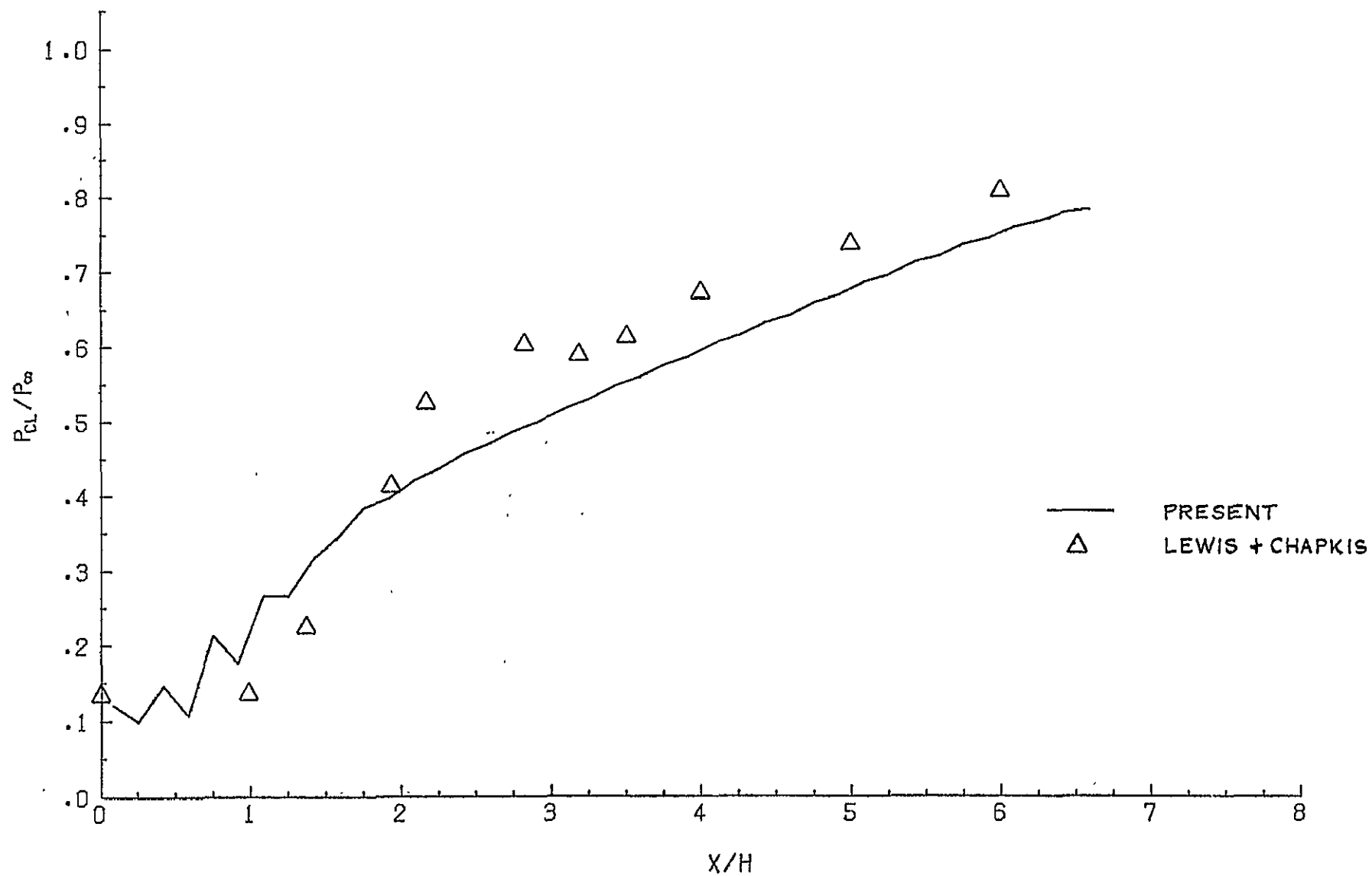


Figure 22. Centerline pressure distribution. Turbulent flow.

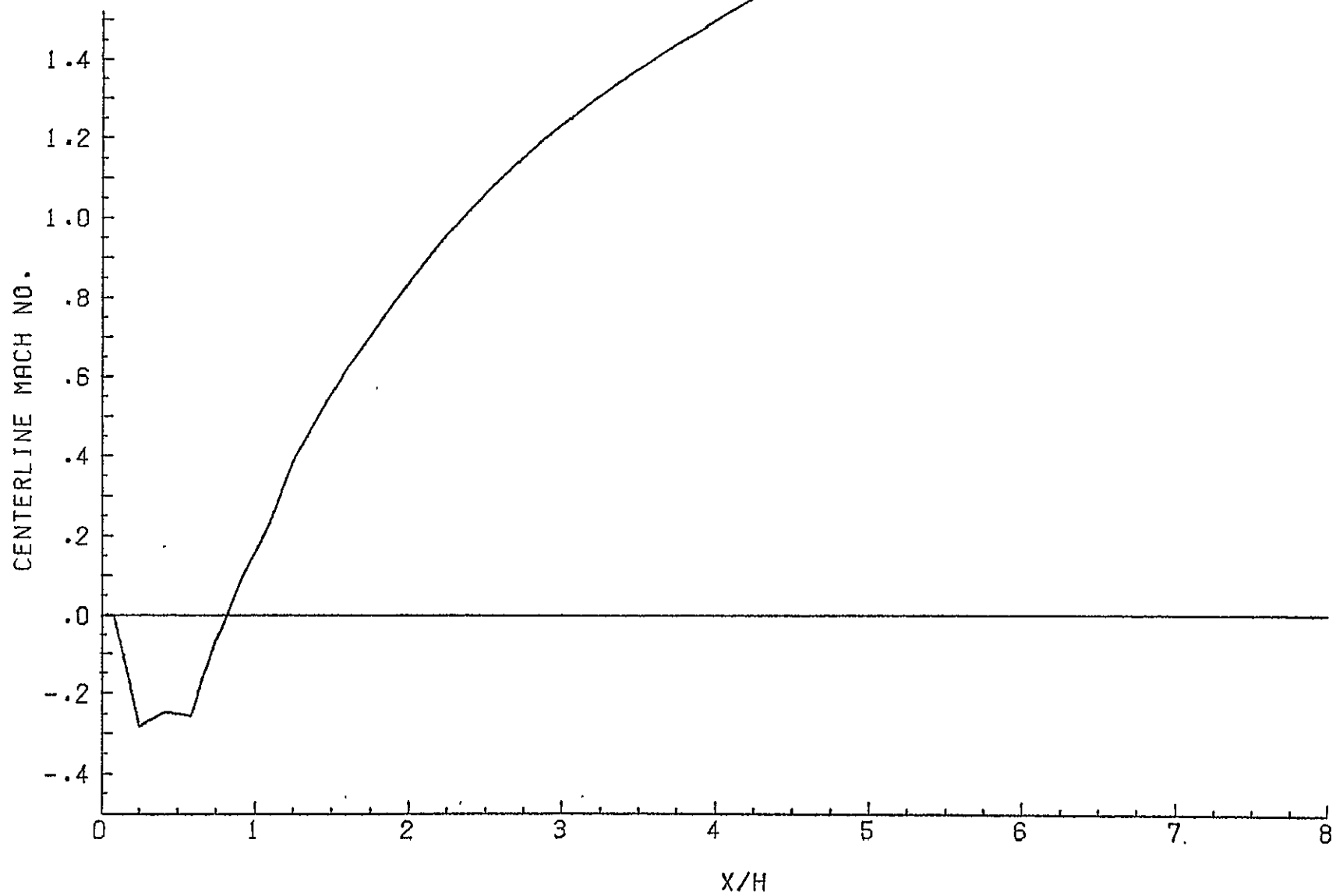


Figure 23. Centerline Mach number distribution. Turbulent flow.

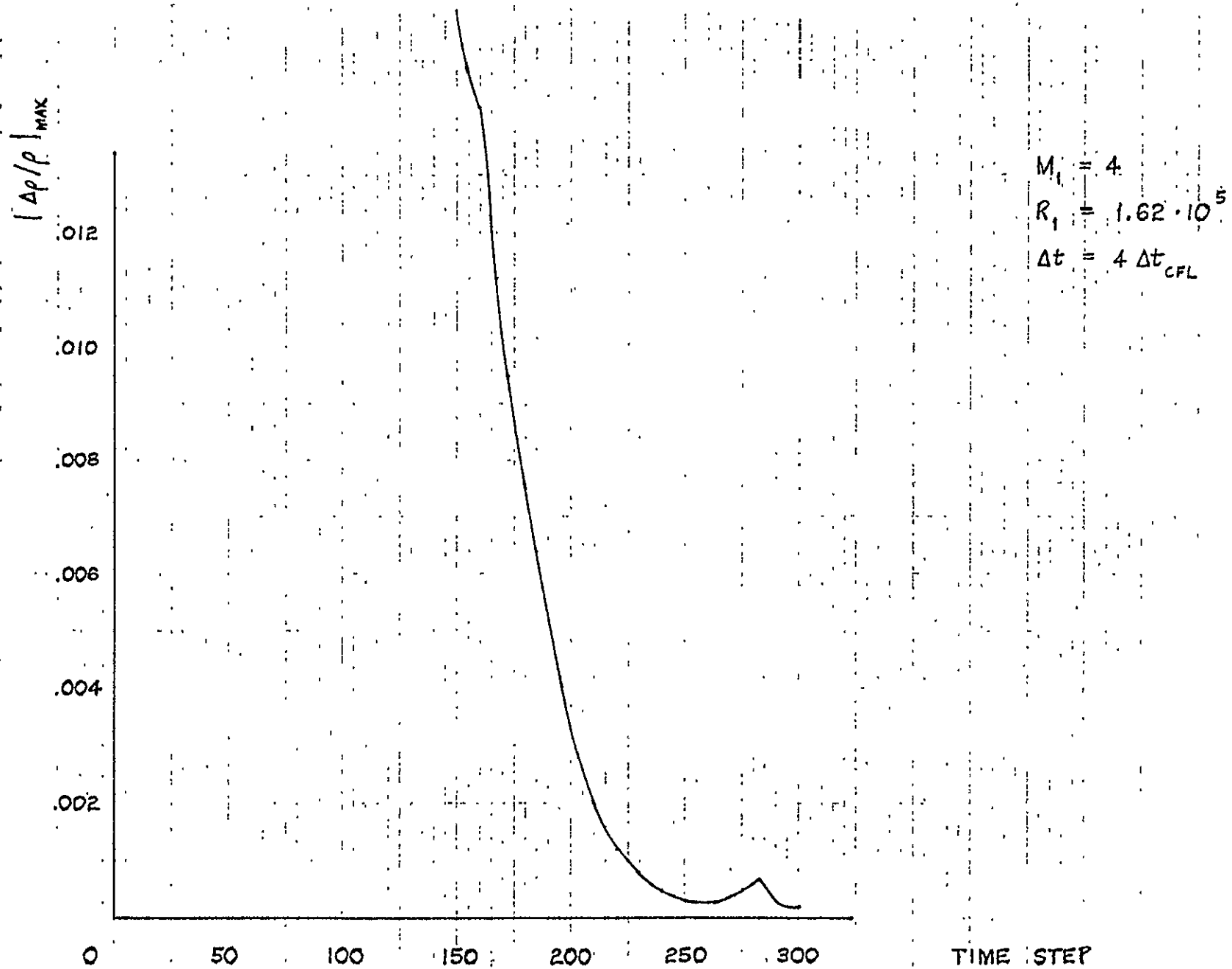


Figure 24. Variation of maximum fractional change in density. Turbulent flow.

Earlier turbulent flow calculations were made at the experimental conditions of Badrinarayanan.⁶ These were $M_1 = 2.07$, $R_1 = 129,000$, and $\delta = 0.55$. The calculated results showed a much larger rise in pressure in the down-stream direction than did the experimental data. Because of the value of M_1 and the grid dimensions, the recompression shock passed through the upper boundary AF near F, instead of through EF as in the preceding cases. After studying the results, it became apparent that the higher pressures were associated with the simple-wave boundary conditions along AF. The left-running compression waves near the shock intersected near AF, in violation of the simple-wave condition. Numerical compression waves were reflected toward the centerline, producing an artificial pressure rise. A possible solution for this is to move AF upward, so that the shock exits through EF. The obvious disadvantage is that more grid points would be required. Alternate boundary conditions are also being considered.

5.0 CONCLUSIONS

(1) The present numerical method computed all of the main features of the supersonic base flows examined, for both the laminar and turbulent cases. These included the corner expansion, the recompression shock, the recirculation region near the base, and the viscous wake near the centerline.

(2) The flow calculations provided a demonstration of the basic stability and convergence of the numerical method.

(3) The numerical results suggest that significant savings in computer time can be achieved, compared with explicit methods, by taking large time steps.

(4) Further study is required to evaluate the effect of the particular two-equation turbulence model being used on the accuracy of the solution. In this connection other turbulence models should also be evaluated.

6.0 REFERENCES

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LIST OF SYMBOLS

A	empirical coefficient in reaction-rate eq. (A20), approximately 12 for the $H_2 - O_2$ reaction
C_a	mean mass fraction of specie a
C_f	mean mass fraction of fuel
C_N	mean mass fraction of N_2
C_O	mean mass fraction of O_2
C_p	mean mass fraction of reaction product
C_μ	empirical coefficient in eq. (A9), approximately 0.09
$C_{\bar{\phi}}$	mean mass fraction of reaction invariant
C_{e1}, C_{e2}	empirical coefficients in ϵ eq. (A16), approximately 1.44 and 1.92, respectively
D_a	molecular diffusion coefficient of specie a
e	mean internal energy per unit mass, made nondimensional by e_1
h_R	heat of reaction per unit mass of fuel, made nondimensional by e_1
H	half-height of base
k	mean turbulent kinetic energy per unit mass, made nondimensional by u_1^2
K	$\gamma(\gamma-1)M_1^2$

M_1	Mach number, $u_1 / [\gamma(\gamma-1)e_1]^{0.5}$
p	mean static pressure, made nondimensional by p_1
Pr	Prandtl number
q_i	$-\partial e / \partial x_i$
R_1	Reynolds number, $\rho_1 u_1 H / \mu_1$
s_{ij}	see eq. (A7)
t	time, made nondimensional by H/u_1
u, v	mean velocity in x- and y-directions, respectively, made nondimensional by u_1
u_i	mean velocity vector, made nondimensional by u_1
u_*	friction velocity, made nondimensional by u_1
$\dot{w}_a$	mean reaction rate of specie a, made nondimensional by u_1/H
x, y, z	Cartesian coordinates, made nondimensional by H
x_i	x, y, z for $i = 1, 2, 3$, respectively
x^+, x^-	right and left edges, respectively, of cell containing grid point ij
y^+, y^-	upper and lower edges, respectively, of cell containing grid point ij

Greek

γ	ratio of specific heats
δ_{ij}	Kronecker delta
δ_x	$(\delta_x \phi)_{ij} = (\phi_{i+1,j} - \phi_{i-1,j})/2\Delta x = (\phi_{x+} - \phi_{x-})/\Delta x$
δ_y	$(\delta_y \phi)_{ij} = (\phi_{i,j+1} - \phi_{i,j-1})/2\Delta y = (\phi_{y+} - \phi_{y-})/\Delta y$
Δt	computational time step, made nondimensional by H/u_1
$\Delta x, \Delta y, \Delta z$	dimensions of cell containing grid point ij , made nondimensional by H
ϵ	dissipation rate of turbulent kinetic energy per unit mass, made nondimensional by u_1^3/H
K	von Karman constant, approximately 0.43
μ	molecular viscosity, made nondimensional by μ_1
μ_T	eddy viscosity, made nondimensional by $\rho_1 u_1 H$
ρ	mean density, made nondimensional by ρ_1
σ_c	turbulent Schmidt number, approximately 0.7
σ_h	turbulent Prandtl number, approximately 0.7
σ_k	empirical coefficient in k-eq., approximately 1.0
σ_ϵ	empirical coefficient in ϵ -eq., approximately 1.3
ϕ	any dependent variable

Subscript

l denotes free stream conditions

Superscripts

n known time level

n+1 unknown time level

* intermediate time level after x-sweep

** time level after y-sweep, taken to be the same as (n+1)

APPENDIX A. Finite Difference Forms of the Conservation Equations

Conservation of Mass

The differential equation for conservation of mass is, using Cartesian tensor notation:

$$\partial \rho / \partial t + \partial \rho u_i / \partial x_i = 0 \quad (A1)$$

This equation is then integrated over a control volume (CV) which is a cell of dimensions Δx , Δy , Δz . Thus,

$$\begin{aligned} \iiint_{CV} (\partial \rho / \partial t) dV &= - \iiint_{CV} (\partial \rho u_i / \partial x_i) dV \\ &= - \iint_{CS} \rho u_i n_i dA \end{aligned} \quad (A2)$$

using Gauss' theorem. For two-dimensional flow, the area integral over the control surface (CS) becomes:

$$\begin{aligned} \iint_{CS} \rho u_i n_i dA &= \iint_{x+} \rho u dy dz + \iint_{x-} \rho u (-1) dy dz \\ &+ \iint_{y+} \rho v dx dz + \iint_{y-} \rho v (-1) dx dz \end{aligned} \quad (A3)$$

Next, the following approximations are made:

$$\begin{aligned} \iiint_{CV} (\partial \rho / \partial t) dV &\cong (\partial \rho / \partial t)_{ij} \cdot \Delta x \cdot \Delta y \cdot \Delta z \\ \iint_{x+} \rho u dy dz &\cong (\rho u)_{x+} \cdot \Delta y \cdot \Delta z \end{aligned} \quad (A4)$$

etc.

Equation (A2) then becomes:

$$(\partial \rho / \partial t)_{ij} = - (1/\Delta x) [(\rho u)_{x+} - (\rho u)_{x-}] - (1/\Delta y) [(\rho v)_{y+} - (\rho v)_{y-}] \quad (A5a)$$

or

$$\partial \rho / \partial t = - \delta_x (\rho u) - \delta_y (\rho v) \quad (A5b)$$

Conservation of Momentum:

The differential equation is:

$$\begin{aligned} \partial(\rho u_i)/\partial t = & - (\partial/\partial x_j) \left\{ \rho u_i u_j + (1/\gamma M_1^2) \rho e \delta_{ij} - (\mu_T + \mu/R_1) s_{ij} \right. \\ & \left. + (2/3) \rho k \delta_{ij} \right\} \end{aligned} \quad (A6)$$

Here,

$$s_{ij} = \partial u_i / \partial x_j + \partial u_j / \partial x_i - (2/3) \delta_{ij} \partial u_m / \partial x_m \quad (A7)$$

and the Reynolds stress tensor is modeled by:

$$\tau_{T,ij} = \mu_T s_{ij} - (2/3) \rho k \delta_{ij} \quad (A8)$$

where

$$\mu_T = C_\mu \rho k^2 / \epsilon \quad (A9)$$

Equation (A6) is next integrated over the control volume that is the cell surrounding grid point (ij). After applying Gauss' theorem and making approximations like those in eqs. (A4), the resulting equations for x- and y-momentum are:

x-momentum:

$$\begin{aligned} \partial \rho u / \partial t = & - \delta_x \left\{ \rho u^2 + \rho e / \gamma M_1^2 - (\mu_T + \mu / R_1) s_{xx} + (2/3) \rho k \right\} \\ & - \delta_y \left\{ \rho u v - (\mu_T + \mu / R_1) s_{xy} \right\} \end{aligned} \quad (A10)$$

y-momentum:

$$\begin{aligned} \partial \rho v / \partial t = & - \delta_x \left\{ \rho u v - (\mu_T + \mu / R_1) s_{xy} \right\} \\ & - \delta_y \left\{ \rho v^2 + \rho e / \gamma M_1^2 - (\mu_T + \mu / R_1) s_{yy} + (2/3) \rho k \right\} \end{aligned} \quad (A11)$$

From eq. (A7),

$$s_{xx} = (4/3) \partial u / \partial x - (2/3) \partial v / \partial y$$

$$s_{xy} = \partial u / \partial y + \partial v / \partial x$$

$$s_{yy} = (4/3) \partial v / \partial y - (2/3) \partial u / \partial x$$

Conservation of Energy

The differential equation is:

$$\begin{aligned} & (\partial / \partial t) \left[\rho e + \rho C_f h_R + (K/2) \rho u_i u_i \right] \\ = & - (\partial / \partial x_j) \left\{ \rho u_j \left[\gamma e + C_f h_R + (K/2) u_i u_i \right] + (\mu_T / \sigma_h + \mu / Pr \cdot R_1) \gamma q_j \right. \\ & \left. - K(\mu_T + \mu / R_1) s_{ij} u_i + (2/3) K \rho k u_j \right\} \\ & + K \rho e - K \mu_T s_{ij} \partial u_i / \partial x_j + (2/3) K \rho k \partial u_i / \partial x_i \end{aligned} \quad (A12)$$

Equation (A12) can be put into finite-difference form by following the same sequence of steps used for conservation of mass and momentum. The result is as follows:

$$\begin{aligned}
 & (\partial/\partial t) \left[\rho e + \rho C_f h_R + (K/2) \rho (u^2 + v^2) \right] \\
 = & - \delta_x \left\{ \rho e \left[\gamma e + C_f h_R + (K/2) (u^2 + v^2) \right] + (\mu_T/\sigma_h + \mu/Pr.R_1) \gamma q_x \right. \\
 & \left. - K(\mu_T + \mu/R_1) s_{ix} u_i + (2/3) K \rho k u \right\} \\
 & - \delta_y \left\{ \rho v \left[\gamma e + C_f h_R + (K/2) (u^2 + v^2) \right] + (\mu_T/\sigma_h + \mu/Pr.R_1) \gamma q_y \right. \\
 & \left. - K(\mu_T + \mu/R_1) s_{iy} u_i + (2/3) K \rho k v \right\} \\
 & + K \rho e - K \mu_T s_{ij} \partial u_i / \partial x_j + (2/3) K \rho k (\partial u / \partial x + \partial v / \partial y) \quad (A13)
 \end{aligned}$$

In equation (A13), the following have been used:

$$q_x = - \partial e / \partial x$$

$$q_y = - \partial e / \partial y$$

$$s_{ix} u_i = \left[(4/3) \partial u / \partial x - (2/3) \partial v / \partial y \right] u + (\partial u / \partial y + \partial v / \partial x) v$$

$$s_{iy} u_i = \left[(4/3) \partial v / \partial y - (2/3) \partial u / \partial x \right] v + (\partial u / \partial y + \partial v / \partial x) u$$

$$s_{ij} \partial u_i / \partial x_j = (4/3) \left[(\partial u / \partial x)^2 - (\partial u / \partial x)(\partial v / \partial y) + (\partial v / \partial y)^2 \right] \\ + (\partial u / \partial y + \partial v / \partial x)^2$$

Conservation of k

The differential equation is:

$$\partial(\rho k) / \partial t = - (\partial / \partial x_j) \left[\rho u_j k - (\mu_T / \sigma_k) (\partial k / \partial x_j) \right] - \rho \epsilon \\ + \mu_T s_{ij} \partial u_i / \partial x_j - (2/3) \rho k \partial u_i / \partial x_i \quad (A14)$$

After following the sequence of steps described in the preceding, the corresponding finite-difference form is:

$$\partial(\rho k) / \partial t = - \delta_x \left[\rho u k - (\mu_T / \sigma_k) (\partial k / \partial x) \right] \\ - \delta_y \left[\rho v k - (\mu_T / \sigma_k) (\partial k / \partial y) \right] - \rho \epsilon \\ + \mu_T s_{ij} \partial u_i / \partial x_j - (2/3) \rho k (\partial u / \partial x + \partial v / \partial y) \quad (A15)$$

Conservation of ϵ

The differential equation is:

$$\partial(\rho \epsilon) / \partial t = - (\partial / \partial x_j) \left[\rho u_j \epsilon - (\mu_T / \sigma_\epsilon) (\partial \epsilon / \partial x_j) \right] \\ + C_{\epsilon 1} (\epsilon / k) \left[\mu_T s_{ij} \partial u_i / \partial x_j - (2/3) \rho k \partial u_i / \partial x_i \right] - C_{\epsilon 2} \rho \epsilon^2 / k \quad (A16)$$

The corresponding finite-difference equation is:

$$\begin{aligned} \partial(\rho\epsilon)/\partial t = & -\delta_x \left[\rho u \epsilon - (\mu_T/\sigma_\epsilon)(\partial\epsilon/\partial x) \right] - \delta_y \left[\rho v \epsilon - (\mu_T/\sigma_\epsilon)(\partial\epsilon/\partial y) \right] \\ & + C_{\epsilon 1} (\epsilon/k) \left[\mu_T s_{ij} \frac{\partial u_i}{\partial x_j} - (2/3) \rho k (\partial u/\partial x + \partial v/\partial y) \right] + C_{\epsilon 2} \rho \epsilon^2/k \end{aligned} \quad (A17)$$

Conservation of Chemical Specie m

The differential equation is:

$$\partial(\rho C_m)/\partial t = -(\partial/\partial x_j) \left[\rho u_j C_m - (\mu_T/\sigma_c + \rho D_m)(\partial C_m/\partial x_j) \right] + \rho \dot{w}_m \quad (A18)$$

The corresponding finite-difference equation is:

$$\begin{aligned} \partial(\rho C_m)/\partial t = & -\delta_x \left[\rho u C_m - (\mu_T/\sigma_c + \rho D_m)(\partial C_m/\partial x) \right] \\ & - \delta_y \left[\rho v C_m - (\mu_T/\sigma_c + \rho D_m)(\partial C_m/\partial y) \right] + \rho \dot{w}_m \end{aligned} \quad (A19)$$

When C_m is C_f , $\dot{w}_f$ can be represented by⁴:

$$\dot{w}_f = -A(\epsilon/k) C_f C_o \quad (A20)$$

When C_m is C_ϕ , then $\dot{w}_f$ is zero.

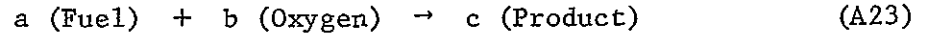
C_o is then computed from:

$$C_o = C_\phi + \lambda C_f \quad (A21)$$

where

$$\lambda = b \hat{w}_o / a \hat{w}_f \quad (\text{A22})$$

and a and b are stoichiometric coefficients for the reaction:



For example, for the $\text{H}_2 - \text{O}_2$ reaction, $\lambda = 8$.

When the oxidizing medium is air, C_N can be computed from:

$$C_N = 1.88 \hat{w}_N \left[(1 - C_f - C_o) \hat{w}_o + 2 C_o \hat{w}_p \right] / \hat{w}_o (\hat{w}_p + 1.88 \hat{w}_N) \quad (\text{A24})$$

Then, C_p is given by:

$$C_p = 1 - C_f - C_o - C_N \quad (\text{A25})$$

APPENDIX B. The Form of the Conservation Equations for the Alternating Direction Implicit (ADI) Solution

Conservation of Mass

A backward time-difference approximation is applied to equation (A5), and then the right-hand side is linearized about the n th time level. The result is:

$$\begin{aligned}
 (\rho^{n+1} - \rho^n)/\Delta t = & -\delta_x(\rho_u^{n,n+1} + \rho^{n+1}_u{}^n - \rho_u^{n,n}) \\
 & -\delta_y(\rho_v^{n,n+1} + \rho^{n+1}_v{}^n - \rho_v^{n,n})
 \end{aligned} \tag{B1}$$

This result is also given as equation (2-5).

For the x-sweep equations, $(n+1)$ th level quantities are evaluated at an intermediate time level, denoted by $*$, except for arguments of δ_y .

$$(\rho^* - \rho)/\Delta t = -\delta_x(\rho^*_u + \rho u^* - \rho u) - \delta_y(\rho v) \tag{B2}$$

(x-sweep)

Here and in what follows, quantities without a superscript are understood to be at the n th level.

The y-sweep equation is formed from equation (B1) by evaluating $(n+1)$ th level quantities at $**$, except for arguments of δ_x , in which $(n+1)$ level quantities are evaluated at $*$.

$$(\rho^{**} - \rho)/\Delta t = -\delta_x(\rho^*_u + \rho u^* - \rho u) - \delta_y(\rho^{**}_v + \rho v^{**} - \rho v) \tag{B3}$$

The final y-sweep equation is obtained by subtracting equation (B2) from equation (B3).

$$(\rho^{**} - \rho^*)/\Delta t = -\delta_y(\rho^{**}v + \rho v^{**} - 2\rho v) \quad (B4)$$

(y-sweep)

Equations (B2) - (B4) also appear as equations (2-7) - (2-9), respectively.

Quantities with superscript ** are considered to be the same as the corresponding quantities at the (n+1)th level.

Conservation of x-Momentum

After time differencing and time linearization, equation (A10) becomes:

$$\begin{aligned} & (\rho^{n+1}u + \rho u^{n+1} - 2\rho u)/\Delta t \\ &= -\delta_x \left[\rho^{n+1}u^2 + 2\rho u^{n+1} - 2\rho u^2 + (\rho^{n+1}e + \rho e^{n+1} - \rho e)/\gamma M_1^2 \right. \\ & \quad \left. - (\mu_T + \mu/R_1) s_{xx}^{n+1} + (2/3)(\rho^{n+1}k + \rho k^{n+1} - \rho k) \right] \\ & - \delta_y \left[\rho^{n+1}uv + \rho u^{n+1}v + \rho uv^{n+1} - 2\rho uv - (\mu_T + \mu/R_1) s_{xy}^{n+1} \right] \end{aligned} \quad (B5)$$

Note that μ_T and μ are evaluated at the nth level, and thus treated explicitly rather than implicitly. The x-sweep equation is:

$$\begin{aligned} & (\rho^*u + \rho u^* - 2\rho u)/\Delta t \\ &= -\delta_x \left\{ \rho^*u^2 + 2\rho u^* - 2\rho u^2 + (\rho^*e + \rho e^* - \rho e)/\gamma M_1^2 \right. \\ & \quad \left. - (\mu_T + \mu/R_1) \left[(4/3)\delta_x u^* - (2/3)\delta_y v \right] + (2/3)(\rho^*k + \rho k^* - \rho k) \right\} \\ & - \delta_y \left[\rho uv - (\mu_T + \mu/R_1) s_{xy} \right] \end{aligned} \quad (B6)$$

Mixed derivatives $\delta_x \delta_y$ are treated explicitly at the nth level, because they are awkward to treat implicitly. The y-sweep equation is:

$$\begin{aligned}
 & (\rho^{**} u + \rho u^{**} - \rho^* u - \rho u^*) / \Delta t \\
 = & - \delta_y \left[\rho^{**} u v + \rho u^{**} v + \rho u v^{**} - 3 \rho u v - (\mu_T + \mu/R_1) \delta_y (u^{**} - u) \right] \quad (B7)
 \end{aligned}$$

Conservation of y-Momentum

The time-linearized difference equation is:

$$\begin{aligned}
 & (\rho^{n+1} v + \rho v^{n+1} - 2 \rho v) / \Delta t \\
 = & - \delta_x \left[\rho^{n+1} u v + \rho u^{n+1} v + \rho u v^{n+1} - 2 \rho u v - (\mu_T + \mu/R_1) s_{xy} \right] \\
 & - \delta_y \left[\rho^{n+1} v^2 + 2 \rho v v^{n+1} - 2 \rho v^2 + (\rho^{n+1} e + \rho e^{n+1} - \rho e) / \gamma M_1^2 \right. \\
 & \quad \left. - (\mu_T + \mu/R_1) s_{yy}^{n+1} + (2/3) (\rho^{n+1} k + \rho k^{n+1} - \rho k) \right] \quad (B8)
 \end{aligned}$$

The x-sweep equation is:

$$\begin{aligned}
& (\rho^* v + \rho v^* - 2 \rho v) / \Delta t \\
& = - \delta_x \left[\rho^*_{uv} + \rho u^* v + \rho_{uv}^* - 2 \rho_{uv} - (\mu_T + \mu/R_1) (\delta_y u + \delta_x v^*) \right] \\
& \quad - \delta \left\{ \rho v^2 + \rho e / \gamma M_1^2 - (\mu_T + \mu/R_1) \left[(4/3) \delta_y v - (2/3) \delta_x u \right] \right. \\
& \quad \left. + (2/3) \rho k \right\} \tag{B9}
\end{aligned}$$

The y-sweep equation is:

$$\begin{aligned}
& (\rho^{**} v + \rho v^{**} - \rho^* v - \rho v^*) / \Delta t \\
& = - \delta_y \left[\rho^{**} v^2 + 2 \rho v v^{**} - 3 \rho v^2 + (\rho^{**} e + \rho e^{**} - 2 \rho e) / \gamma M_1^2 \right. \\
& \quad \left. - (\mu_T + \mu/R_1) (4/3) \delta_y (v^{**} - v) + (2/3) (\rho^{**} k + \rho k^{**} - 2 \rho k) \right] \tag{B10}
\end{aligned}$$

Conservation of Energy

The time-linearized difference equation is:

$$\begin{aligned}
 & (1/\Delta t) \left\{ \rho^{n+1} \left[e + C_f h_R + (K/2) (u^2 + v^2) \right] + \rho(e^{n+1} + C_f^{n+1} h_R) \right. \\
 & \quad \left. + K\rho(uu^{n+1} + vv^{n+1}) - 2\rho(e + C_f h_R) - (3/2)K\rho(u^2 + v^2) \right\} \\
 & = - \delta_x \left\{ (\rho^{n+1} u + \rho u^{n+1}) \left[\gamma e + C_f h_R + (K/2) (u^2 + v^2) \right] \right. \\
 & \quad + \rho u (\gamma e^{n+1} + C_f^{n+1} h_R + Kuu^{n+1} + Kvv^{n+1}) \\
 & \quad - \rho u \left[2(\gamma e + C_f h_R) + (3/2) K (u^2 + v^2) \right] \\
 & \quad - (\mu_T/\sigma_h + \mu/Pr \cdot R_1) \gamma \delta_x e^{n+1} \\
 & \quad \left. - K(\mu_T + \mu/R_1) s_{ix} u_i + (2/3) K \rho k u \right\} \\
 & - \delta_y \left\{ (\rho^{n+1} v + \rho v^{n+1}) \left[\gamma e + C_f h_R + (K/2) (u^2 + v^2) \right] \right. \\
 & \quad + \rho v (\gamma e^{n+1} + C_f^{n+1} h_R + Kuu^{n+1} + Kvv^{n+1}) \\
 & \quad - \rho v \left[2(\gamma e + C_f h_R) + (3/2) K (u^2 + v^2) \right] \\
 & \quad - (\mu_T/\sigma_h + \mu/Pr \cdot R_1) \gamma \delta_y e^{n+1} \\
 & \quad \left. - K(\mu_T + \mu/R_1) s_{iy} u_i + (2/3) K \rho k v \right\} \\
 & + K\rho e - K \mu_T s_{ij} \partial u_i / \partial x_j + (2/3) K \rho k (\delta_x u + \delta_y v) \tag{B11}
 \end{aligned}$$

The production and dissipation terms have been treated explicitly at the n th level.

The x-sweep energy equation is:

$$\begin{aligned}
& (1/\Delta t) \left\{ \rho^* \left[e + C_f h_R + (K/2) (u^2 + v^2) \right] + \rho (e^* + C_f^* h_R) \right. \\
& \quad \left. + K\rho (uu^* + vv^*) - 2\rho(e + C_f h_R) - (3/2) K\rho(u^2 + v^2) \right\} \\
& = - \delta_x \left\{ (\rho^* u + \rho u^*) \left[\gamma e + C_f h_R + (K/2)(u^2 + v^2) \right] \right. \\
& \quad \left. + \rho u (\gamma e^* + C_f^* h_R + Kuu^* + Kvv^*) \right. \\
& \quad \left. - \rho u \left[2(\gamma e + C_f h_R) + (3/2)K(u^2 + v^2) \right] \right. \\
& \quad \left. - (\mu_T/\sigma_h + \mu/Pr \cdot R_1) \gamma \delta_x e^* \right. \\
& \quad \left. - K(\mu_T + \mu/R_1) s_{ix} u_i + (2/3) K\rho k u \right\} \\
& - \delta_y \left\{ \rho v \left[\gamma e + C_f h_R + (K/2)(u^2 + v^2) \right] \right. \\
& \quad \left. - (\mu_T/\sigma_h + \mu/Pr \cdot R_1) \gamma \delta_y e \right. \\
& \quad \left. - K(\mu_T + \mu/R_1) s_{iy} u_i + (2/3) K\rho k v \right\} \\
& + K\rho e - K\mu_T s_{ij} \partial u_i / \partial x_j + (2/3) K\rho k (\delta_x u + \delta_y v) \tag{B12}
\end{aligned}$$

The y-sweep energy equation is:

$$\begin{aligned}
 (1/\Delta t) & \left\{ (\rho^{**} - \rho^*) \left[e + C_f h_R + (K/2) (u^2 + v^2) \right] + \rho (e^{**} - e^*) \right. \\
 & \left. + \rho (C_f^{**} - C_f^*) h_R + K\rho \left[u(u^{**} - u^*) + v(v^{**} - v^*) \right] \right\} \\
 = & -\delta_y \left\{ (\rho^{**} v + \rho v^{**}) \left[\gamma e + C_f h_R + (K/2) (u^2 + v^2) \right] \right. \\
 & + \rho v (\gamma e^{**} + C_f^{**} h_R + K u u^{**} + K v v^{**}) \\
 & - \rho v \left[3(\gamma e + C_f h_R) + 2K(u^2 + v^2) \right] \\
 & \left. - (\mu_T/\sigma_h + \mu/Pr.R_1) \gamma \delta_y (e^{**} - e) \right\} \quad (B13)
 \end{aligned}$$

Conservation of k

The time-linearized difference equation is:

$$\begin{aligned}
 & (\rho^{n+1} k + \rho k^{n+1} - 2\rho k)/\Delta t \\
 = & -\delta_x \left[\rho^{n+1} u k + \rho u^{n+1} k + \rho u k^{n+1} - 2\rho u k - (\mu_T/\sigma_k) \delta_x k^{n+1} \right] \\
 & - \delta_y \left[\rho^{n+1} v k + \rho v^{n+1} k + \rho v k^{n+1} - 2\rho v k - (\mu_T/\sigma_k) \delta_y k^{n+1} \right] \\
 & - \rho e + \mu_T s_{ij} \partial u_i / \partial x_j - (2/3)\rho k (\delta_x u + \delta_y v) \quad (B14)
 \end{aligned}$$

The x-sweep k-equation is:

$$\begin{aligned}
 & (\rho^* k + \rho k^* - 2\rho k) / \Delta t \\
 & = - \delta_x \left[\rho^* u k + \rho u^* k + \rho u k^* - 2\rho u k - (\mu_T / \sigma_k) \delta_x k^* \right] \\
 & \quad - \delta_y \left[\rho v k - (\mu_T / \sigma_k) \delta_y k \right] - \rho \epsilon + \mu_T s_{ij} \partial u_i / \partial x_j \\
 & \quad - (2/3) \rho k (\delta_x u + \delta_y v)
 \end{aligned} \tag{B15}$$

The y-sweep k-equation is:

$$\begin{aligned}
 & \left[(\rho^{**} - \rho^*) k + \rho (k^{**} - k) \right] / \Delta t \\
 & = - \delta_y \left[\rho^{**} v k + \rho v^{**} k + \rho v k^{**} - 3\rho v k - (\mu_T / \sigma_k) \delta_y (k^{**} - k) \right]
 \end{aligned} \tag{B16}$$

Conservation of ϵ

The time-linearized difference equation is:

$$\begin{aligned}
 & (\rho^{n+1} \epsilon + \rho \epsilon^{n+1} - 2\rho \epsilon) / \Delta t \\
 & = - \delta_x \left[\rho^{n+1} u \epsilon + \rho u^{n+1} \epsilon + \rho u \epsilon^{n+1} - 2\rho u \epsilon - (\mu_T / \sigma_\epsilon) \delta_x \epsilon^{n+1} \right] \\
 & \quad - \delta_y \left[\rho^{n+1} v \epsilon + \rho v^{n+1} \epsilon + \rho v \epsilon^{n+1} - 2\rho v \epsilon - (\mu_T / \sigma_\epsilon) \delta_y \epsilon^{n+1} \right] \\
 & \quad + C_{\epsilon 1} (\epsilon / k) \left[\mu_T s_{ij} \partial u_i / \partial x_j - (2/3) \rho k (\delta_x u + \delta_y v) \right] - C_{\epsilon 2} \rho \epsilon^2 / k
 \end{aligned} \tag{B17}$$

The x-sweep ϵ -equation is:

$$\begin{aligned}
 & (\rho^* \epsilon + \rho \epsilon^* - 2\rho\epsilon)/\Delta t \\
 & = - \delta_x \left[\rho^* u \epsilon + \rho u^* \epsilon + \rho u \epsilon^* - 2\rho u \epsilon - (\mu_T/\sigma_\epsilon) \delta_x \epsilon^* \right] \\
 & \quad - \delta_y \left[\rho v \epsilon - (\mu_T/\sigma_\epsilon) \delta_y \epsilon \right] \\
 & + C_{e1} (\epsilon/k) \left[\mu_T s_{ij} \partial u_i / \partial x_j - (2/3) \rho k (\delta_x u + \delta_y v) \right] - C_{e2} \rho \epsilon^2 / k \quad (B18)
 \end{aligned}$$

The y-sweep ϵ -equation is:

$$\begin{aligned}
 & \left[(\rho^{**} - \rho^*) \epsilon + \rho (\epsilon^{**} - \epsilon^*) \right] / \Delta t \\
 & = - \delta_y \left[\rho^{**} v \epsilon + \rho v^{**} \epsilon + \rho v \epsilon^{**} - 3\rho v \epsilon - (\mu_T/\sigma_\epsilon) \delta_y (\epsilon^{**} - \epsilon) \right] \quad (B19)
 \end{aligned}$$

Conservation of Species

The time-linearized difference equation is:

$$\begin{aligned}
& (\rho^{n+1} C_a + \rho C_a^{n+1} - 2\rho C_a)/\Delta t \\
& = - \delta_x \left[\rho^{n+1} u C_a + \rho u^{n+1} C_a + \rho u C_a^{n+1} - 2 \rho u C_a \right. \\
& \quad \left. - (\mu_T/\sigma_c + \rho D_a) \delta_x C_a^{n+1} \right] \\
& - \delta_y \left[\rho^{n+1} v C_a + \rho v^{n+1} C_a + \rho v C_a^{n+1} - 2 \rho v C_a - (\mu_T/\sigma_c + \rho D_a) \delta_y C_a^{n+1} \right] \\
& \quad + \rho \dot{w}_a \tag{B20}
\end{aligned}$$

The x-sweep species conservation equations is:

$$\begin{aligned}
& (\rho^* C_a + \rho C_a^* - 2 \rho C_a)/\Delta t \\
& = - \delta_x \left[\rho^* u C_a + \rho u^* C_a + \rho u C_a^* - 2 \rho u C_a - (\mu_T/\sigma_c + \rho D_a) \delta_x C_a^* \right] \\
& \quad - \delta_y \left[\rho v C_a - (\mu_T/\sigma_c + \rho D_a) \delta_y C_a \right] + \rho \dot{w}_a \tag{B21}
\end{aligned}$$

The y-sweep species conservation equation is:

$$\begin{aligned}
& \left[(\rho^{**} - \rho^*) C_a + \rho (C_a^{**} - C_a^*) \right]/\Delta t \\
& = - \delta_y \left[\rho^{**} v C_a + \rho v^{**} C_a + \rho v C_a^{**} - 3 \rho v C_a - (\mu_T/\sigma_c + \rho D_a) \delta_y (C_a^{**} - C_a) \right] \\
& \tag{B22}
\end{aligned}$$